

### **§3. Stretching Grains—"Small Strain" Creep as an "Elastic" Deformation**

"*Small strain*" creep means the sort that might be presumed. Specimen strains are small,  $\varepsilon < 0.1$ ,  $\varepsilon$  denoting the plastic strain of the bulk material in the tensile specimen, and deformation occurs in such a fashion that the grains deform while maintaining their identities and relative positions: grains "stretch" along the tensile axis, or *longitudinal direction*, and contract along the *transverse directions*; and since the volume of the material does not change during a plastic deformation, *Poisson's ratio*,  $\nu$ , is one-half.

An idealized, three-dimensional cellular array which models the polycrystalline microstructure is a stack of tetrakaidecahedrons. The "dual" lattice to this cellular array is BCC. In two dimensions the cells are hexagons and the "dual" is a lattice with *sixfold symmetry*. The "dual" lattice points deform "elastically" during "small strain" creep; the prior considerations are therefore applicable.

Figure 19 illustrates "diffusional creep," which occurs when grain boundaries move under the action of an applied stress as shown. Grain boundaries respond to stress with two distinct types of motion at high temperatures: *sliding* (parallel to the boundary) and *migrating* (normal to the boundary) (Poirier 1985). Grain boundary sliding is probably the result of *grain boundary dislocation* climb and glide, and these are likely controlled by atomic diffusion (Gates 1973). See Figure 20. Therefore, while grain boundary sliding may occur to some extent at low temperatures  $T$ , it is only prevalent for  $T > 0.4T_m$ , where  $T_m$  is the melting point in degrees Kelvin (Pond, Smith and Southerden 1978). Dislocation interactions, dissociations or associations, permit the propagation of sliding from one grain boundary to another. Dislocation activity for sliding may also produce some level of grain

boundary migration; while grain boundary migration frequently accompanies sliding, these processes do not need to occur simultaneously;<sup>[36]</sup> the "driving force" for ***stress-assisted grain boundary migration*** could be attributable to elastic energy from lattice dislocations piling up against the boundary.

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[36]: Following Pond *et al.* (1978): When a grain boundary is in an orientation where all crystal lattice sites are also sites of the coincidence site lattice (CSL), grain boundary dislocations which have a Burgers vector equal to that of a displacement shift complete (DSC) lattice translation vector move such that both sliding and migration occur. (Bollman (1970) and Hirth and Lothe (1982) define these defects.) When only a fraction,  $i/\Sigma$  of crystal lattice sites are CSL sites ( $i \leq \Sigma$  is an integer) a DSC dislocation need not give simultaneous grain boundary sliding and migration; but there is a relationship between sliding and migration that is dependent on the Burgers vector of the dislocation and the grain boundary orientation. See also Ashby (1972).

### 3.1. Compatibility

Creep of a polycrystalline material by grain boundary sliding with accommodation by atomic diffusion is "true" *diffusional creep* (Raj and Ashby 1971).<sup>[37]</sup> Alternatively, grain boundary movement occurs as a consequence of the atomic diffusion which elongates the grains (Langdon 1970) so that matter is *compatibly* redistributed throughout the material: in other words grain boundary sliding and migration *accommodate* atomic diffusion.

Grain boundary sliding has been viewed as only an accommodation mechanism for diffusional creep, but Steven's (1971) suggests that in order to maintain grain compatibility,

$$\dot{\varepsilon}_G \approx \dot{\varepsilon}_{GBS}/1.6, \quad (1)$$

where  $\dot{\varepsilon}_G$  is the rate at which grains strain and  $\dot{\varepsilon}_{GBS}$  is the strain rate from grain boundary sliding/migration;

$$\dot{\varepsilon}_{GBS} \approx v_{GBS}/d, \quad (2)$$

$v_{GBS}$  is the relative velocity of the two grains and  $d$  is the grain size (Edington *et al.* 1976).

Grain boundary sliding is a thermally activated process:  $v_{GBS} = A\exp(-Q_{GBS}/kT)\tau$ . Here,

$A$  is a constant,  $Q_{GBS}$  is an activation energy,  $k$  is Boltzmann's constant, and  $\tau$  is the resolved stress in the grain boundary; the quantity  $A\exp(-Q_{GBS}/kT)$  can be taken as  $\delta/\eta$ , where  $\delta$  is the

[37]: The grain boundary migration which accompanies sliding may also produce grain growth (Raj and Ashby 1971).

grain boundary width and  $\eta$  the grain boundary viscosity (Cottrell 1953). *Grain compatibility* means that relative grain boundary motions do not produce gaps in the material.

The *grain strain rate* is the sum of the strain rates from processes that plastically deform the grains:

$$\dot{\varepsilon}_G = \dot{\varepsilon}_{\text{diff.}} + \dot{\varepsilon}_{\text{dislo.}}, \quad (3)$$

where  $\dot{\varepsilon}_{\text{diff.}}$  is the strain rate from diffusional creep and  $\dot{\varepsilon}_{\text{dislo.}}$  is the strain rate from dislocation creep. The *total strain rate*,  $\dot{\varepsilon}$ , is (Langdon 1970)

$$\dot{\varepsilon} = \dot{\varepsilon}_G + \dot{\varepsilon}_{\text{GBS}}. \quad (4)$$

It is generally assumed that diffusional creep results in grain strain (Ashby and Verrall 1973); but Rachinger (1952-53), Beeré (1976) and Spingarn and Nix (1978) all suggest that grain rearrangements, *i.e.* neighbor switching, may occur during diffusional creep, resulting in the retention of an equiaxed microstructure, as opposed to producing grain strain. Grain rearrangements are, however, not the subject of this section; they will be discussed later on in relationship to superplastic deformation.

*Dislocation creep* tends to occur at higher strain rates than diffusional creep. Polycrystalline materials also undergo grain boundary sliding during dislocation creep, and in this case sliding concentrates stress at grain corners (or triple points) (Beeré 1978); see also Ishida, Mullendore and Grant (1965).

### 3.2. Dislocations

There is a complete analogy between the lattice dislocations introduced earlier and the *cellular dislocations*, Figure 21, in a "regular" array of cells (Morral and Ashby 1974). Introduction of non-hexagonal cells in a honeycomb array produces "strain energy" because the cells have surface tension and irregular cells increase the amount of boundary length per unit area.

#### 3.2.1. The Shear Modulus

An "ideal" soap froth has no shear modulus and therefore is always in equilibrium; but this is not the case for metallurgical grains (Weaire and Rivier 1984). Hamilton suggests the following analysis for the shear modulus of a cellular array which models a polycrystalline material. The result is very similar to one from Princen (1983) for foams. Note that the shear modulus calculated here is not mechanical as in, for example, Ashby's (1983) discussion of the mechanical properties of cellular solids. It is instead concerned with the amount of energy which must be supplied to an array of cells to make them stretch during, for example, creep or superplastic deformation.

Consider a hexagonal array as the initial state and cause a distortion to the array by imposing a shear stress. The cells have edge length  $a$ , diameter  $d = 2a$  and width  $b = \sqrt{3}d/2$ . The area of a polygon with  $n$ -sides is  $A_n = \frac{1}{4}na^2\cot[\pi/n]$ . After shear distortion of amount  $\beta$  the area is  $A_n^d = \frac{1}{4}na_d^2\cot[\pi/n]\cos(\beta)$ ,  $A_n^d$  and  $a_d$  denoting the area and edge length of the polygon in the distorted state, respectively. For plane-strain deformation the cell areas are constant,  $A_n = A_n^d$ , and therefore  $a_d = a/[\cos(\beta)]^{1/2}$ . The initial perimeter of the polygon

is  $P_n = na$ ; after distortion it is  $P_n^d = na_d = na/[\cos(\beta)]^{1/2}$ . The differential change in the perimeter length upon distortion is therefore  $\Delta P_n = \frac{1}{2}\{nas\sin(\beta)/[\cos(\beta)]^{3/2}\}\Delta\beta \approx \frac{1}{2}na\beta\Delta\beta$ , the approximation holding for small  $\beta$ . The energy related to this distortion scales with the surface tension  $\Gamma$  (energy per unit area); the cell area is the cell perimeter multiplied by unit depth for a *columnar structure*. Therefore the incremental energy increase associated with the distortion is  $\Delta E_n = \frac{1}{2}na\Gamma\beta\Delta\beta$ , e.g.,  $\Delta E_6 = 3a\Gamma\beta\Delta\beta = 1.5d\Gamma\beta\Delta\beta$  for a hexagon. The number of cells per unit volume for a columnar array of hexagons is  $N_v = 1/(A_6 \times 1) = 1/[3\sqrt{3} (d/2)^2/2] = 1.54/d^2$ . So the energy per unit volume required to deform cells is given by  $\Delta E_{vol} = N_v\Delta E_6 = 2.31[\Gamma/d]\beta\Delta\beta$ . Now compare this to the elastic distortion energy per unit volume,  $\Delta E_{vol}$ , of an isotropic crystal, where the distortion angle  $\beta$  is equal to the shear strain  $\gamma$  as  $\Delta E_{vol} = G\gamma d\gamma$ , where  $G$  denotes the shear modulus. Comparing the expressions  $\Delta E_{vol} = 2.31[\Gamma/d]\beta\Delta\beta$  and  $\Delta E_{vol} = G\gamma d\gamma$  indicates that the shear modulus of the cellular array, say  $\mathbf{G}$ , is  $\mathbf{G} = 2.31[\Gamma/d] = 2\Gamma/b$ . This result is comparable to the Ashby-Verrall (1973) threshold stress,  $\sigma_o \equiv 0.72\Gamma/d$ , required to make grains stretch during creep or superplastic deformation.

### 3.2.2. Topology

The ***structural properties of random tissues*** from Rivier (1985) are as follows:<sup>[38]</sup>

**(1) Elementary Structural Transformations:** There are only two elementary transformations for the cells in an array: T1, or neighbor switching, and T2, or cell disappearance, and their inverses. The first corresponds to cellular dislocation glide and the

[38]: See also any of the citations for Rivier in the Reference section.

second to cellular dislocation climb.

**(2) Structural Stability:** Only vertices with *coordination* (number of edges incident on a given vertex) 3 are allowed in a two dimensional cellular array and 4 in a three dimensional array. Vertices of higher coordination are transformed to these values by neighbor switching.

**(3) Conservation Laws:** There are two: (1) *Euler's relation*,

$$\text{Two Dimensions: } f - e + v = 2,$$

$$\text{Three Dimensions: } c + f - e + v = 0;$$

where  $f \equiv$  *number of faces* (faces are cells in two dimensions),  $e \equiv$  *number of edges*,  $v \equiv$  *number of vertices*,  $c \equiv$  *number of cells*. (2) *Bianchi identity*:<sup>[39]</sup> odd lines are the only topologically stable "extended" constituents. *Odd lines* are "lines" extending through faces (cells in two dimensions) which have an odd number of edges. This means that disclinations (*e.g.* a 5- or 7-sided cell in two dimensions) are always paired, even if they are not adjacent as in the 5-7 combination which makes a dislocation. These laws result in the topological constraints

$$\text{Two Dimensions} \quad \langle n \rangle = 6,$$

$$\text{Three Dimensions} \quad \langle f \rangle = 12/(6 - \langle n \rangle);$$

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[39]: Equivalent to the version presented earlier and discussed in more detail in the Appendix.

here,  $n \equiv$  number of edges per face (or number of edges per cell in two dimensions), and  $\langle \dots \rangle$  denotes the average, or expectation value.

Consider an array of only hexagons (honeycomb array). All cells have six sides,  $n = 6$ . Remove a hexagon and replace it with a pentagon,  $n = 5$ ; bend the cells so that they all fit together without any gaps. The average number of edges per cell is  $\langle n \rangle \equiv \sum_{\text{all cells}} np_n < 6$ , where  $p_n$  is the frequency with which cells having  $n$ -sides are found. In this case the scalar curvature  $R$  from the Riemann curvature tensor  $\mathbf{R}$  is  $R > 0$ . Similarly if a hexagon in a honeycomb array is replaced by a heptagon,  $n = 7$ , then  $\langle n \rangle \equiv \sum_{\text{all cells}} np_n > 6$  and  $R < 0$ . If, on the other hand, irregular cells are introduced into the array only in pairs like 5-7 and 4-8, i.e. as cellular dislocations, then  $\langle n \rangle \equiv \sum_{\text{all cells}} np_n = 6$  and  $\int \mathbf{R} = \mathbf{0}$ .

The cellular dislocation density is proportional to the fraction of non-hexagonal cells,  $X_d$ , in the array (Morral and Ashby 1974). For example, Carnal and Mocellin (1981) write

$$X_d \equiv \frac{1}{2} \sum_{n \geq 3} |n - 6| p_n.$$

The cellular dislocation pair is a convenient object to illustrate compatibility, Figure 22. In this figure all of the dislocations are closed loops so the sum of all the Burgers vectors is zero,  $\int_A T^m_{np} \vec{dx}^n \wedge \vec{dx}^p = 0$  for every cross-section  $A$ , a condition which corresponds to no macroscopic bending (Kosevich 1979),  $\mathbf{R} = \mathbf{0}$  in all regions (i.e. "locally").

**The dislocation strain in a cellular array is revealed by a distribution in the number of grain faces.**

### 3.3. A Discussion of Creep

A *creep mechanism* results from the assumption that a particular process, or accommodation mechanism, is rate limiting, *i.e.* determines, "controls" or "dominates" the strain rate. For *Nabarro-Herring creep* the rate limiting step for diffusional creep is assumed to be atomic diffusion through the lattice, or bulk material in between grain boundaries; while the rate limiting step for *Coble creep* is assumed to be atomic diffusion through the grain boundaries (Poirier 1985). Both of these creep mechanisms predict that the creep, or strain rate,  $\dot{\varepsilon}$ , is proportional to the stress,  $\sigma$ , and therefore that the material is *Newtonian viscous*. The Coble creep rate is proportional to the atomic diffusivity in grain boundaries,  $D_B$ , and inversely proportional to the cube of the grain size; the Nabarro-Herring creep rate is proportional to the lattice diffusivity,  $D_V$ , and inversely proportional to the square of the grain size (Poirier 1985). Thus, Coble creep is more sensitive to the grain size,  $d$ . Atomic diffusion is a thermally activated process:  $D_i = D_{o,i} \exp(-Q_i/kT)$ , where  $D_{o,i}$  is a constant,  $Q_i$  is an activation energy,  $k$  is Boltzmann's constant, and  $i = V$  and  $B$  for lattice (or bulk) and grain boundary diffusion, respectively. Since the activation energy for grain boundary diffusion,  $Q_B$ , is less than that for lattice diffusion,  $Q_V$ , Coble creep dominates at lower deformation temperatures. The strain rate for Coble creep,  $\dot{\varepsilon} \equiv \dot{\varepsilon}_{\text{diff.}}$ , is given by

$$\dot{\varepsilon}_{\text{diff.}} = A \left( \frac{D_B \delta \Omega}{k T d^3} \right) \sigma, \quad (5)$$

where  $\delta$  and  $\Omega$  are respectively the grain boundary "width" and atomic volume, and  $A = 148$

for a tensile stress. The strain rate for Nabarro-Herring creep is given by

$$\dot{\varepsilon}_{\text{diff.}} = A \left( \frac{D_v \Omega}{k T d^2} \right) \sigma, \quad (6)$$

where  $A = 40/3$  for a tensile stress.<sup>[40]</sup> The atomic mobility,  $m_i$  is defined as  $m_i \equiv D_i/kT$ , and therefore the *constitutive relationship* for diffusional creep is  $\dot{\varepsilon} \equiv \dot{\varepsilon}_{\text{diff.}} \propto m_i \sigma / d^\mu$ ;  $\mu = 2$  and  $m_i = m_v = D_v/kT$  for Nabarro-Herring creep, while  $\mu = 3$  and  $m_i = m_B = D_B/kT$  for Coble creep. For both types of diffusional creep, the *crystal strain rate sensitivity*,  $m_c$ , is  $m_c = 1$ . Thus, if only these processes are operative in a material, if the grain size  $d = \text{constant}$ , and if deformation is homogeneous (Zelin *et al.* 1994), *i.e.* all grains deform simultaneously, then the *observed strain rate sensitivity*,  $m$ ,

$$m \equiv d(\ln \sigma) / d(\ln \dot{\varepsilon}),$$

will be  $m = 1$ .

Grain boundary sliding arises because the shear and normal forces acting on the boundaries can be relaxed by separate mechanisms at different rates. Then deformation of the body can become non-uniform, or in-homogeneous (Beeré 1978). In diffusional creep of polycrystalline materials, grain shape changes result from a redistribution of material around the grain boundaries; grain interiors are not plastically deformed, although the atomic

[40]: The constant  $A$  in creep relationships fit to experimental data can be found to be much larger than these predicted values (Beeré 1976).

lattice may rotate (Beeré 1976). Grain boundary sliding and mass transport for diffusional creep are sequential processes such that the slower process will *control* the creep rate. Equations (5) and (6) are developed under the assumption that grain boundary sliding rapidly relaxes shear stresses on the boundaries (easy sliding), and is consequently not rate limiting; these creep rates are therefore controlled by diffusive mass transport. For this case of *easy grain boundary sliding*, boundaries are unable to support shear stresses and only normal boundary stresses support the applied load; grain boundary sliding has a short relaxation time relative to diffusion across the grain (Beeré 1978).

The rate limiting step for diffusional creep is mass transport because grain boundary sliding rapidly releases boundary shear stresses. Relatively rapid grain boundary sliding may result from the much shorter diffusion path between grain boundary dislocations (in comparison to the distance between grain boundaries), as in Figure 23. If, on the other hand, mass transport is rapid, perhaps because the grain size is very small and diffusion distances correspondingly short, and if grain boundary sliding is relatively slow, perhaps because grain boundary dislocations are immobilized, then the creep rate may be controlled by sliding. In this case grain boundaries develop shear stresses and the normal stresses relax to some constant value; deformation is controlled by the sliding mechanism and is accommodated by diffusion. Boundary shear stresses will not all be the same because grain boundaries have different effective viscosities from a number of effects, the most fundamental of which must be crystallographic.

The applied stress does work during grain boundary sliding, and the work rate can be minimized if grains rotate instead of sliding along more viscous boundaries,

Figure 24a. A given strain is attained with minimal energy expenditure, as follows, after Beeré (1978).<sup>[41]</sup>

Figure 24b shows a uniform array of hexagons that will deform by grain boundary sliding and grain rotations. The sliding displacement rate on 'a' boundaries,  $\dot{x}_a$ , is  $\dot{x}_a = \dot{S}_a - \dot{\omega}\sqrt{3}d/2$ , where  $\dot{S}_a \equiv \partial S_a / \partial t$  and  $\dot{\omega}$  are the shear displacement rate and rotation rate, respectively, both relative to the grain center. Since  $S_a + S_b + S_c = 0$ ,  $\dot{x}_a + \dot{x}_b + \dot{x}_c = -3\dot{\omega}\sqrt{3}d/2$ , the grain center shear is consequently  $\dot{S}_a = 1/3(2\dot{x}_a - \dot{x}_b - \dot{x}_c)$ . The strain can be expressed as

$$\varepsilon d = \frac{2}{3}(S_a - S_b)(2\cos^2 \theta - 1) + \frac{4}{3}(S_a + S_b - 2S_c)\sin \theta \cos \theta;$$

thus,

$$\dot{\varepsilon}d = \frac{2}{3}(\dot{x}_a - \dot{x}_b)(2\cos^2 \theta - 1) + \frac{2}{3}(\dot{x}_a + \dot{x}_b - 2\dot{x}_c)(2\sin \theta \cos \theta)/\sqrt{3}, \quad (7)$$

again, assuming that  $d = \text{constant}$  and  $\theta = \text{constant}$ . The strain rate can be determined only after the sliding displacement rates.

Beeré assumes that the sliding rates are proportional to *grain boundary mobility terms*,  $M_a$ , and the resolved shear stress on the boundaries,  $\tau_a$ :

$$\dot{x}_a = M_a \|\boldsymbol{\tau}_a^{g-1} \|\boldsymbol{\tau}_a,$$

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[41]: Beeré uses the hexagon width,  $b$ , as the grain size whereas I use the hexagon diameter,  $d$ ;  $b = \sqrt{3}d/2$ .

where the modulus ensures the correct shear direction when the *stress exponent*,  $\varphi$ , is even.

The mobility terms  $M_a$  are inversely proportional to the grain boundary viscosities,  $\eta_a$ ,  $M_a = \delta/\eta_a$ ,  $\delta$  again denoting the grain boundary width (Cottrell 1953). If all grain boundaries are equally resistant to shear,  $M_a = M_b = M_c \equiv M$ , then for  $\varphi = 1$ , equation (7) gives the creep

rate  $\dot{\varepsilon} \equiv \dot{\varepsilon}_{GBS}$

$$\dot{\varepsilon}_{GBS} = \frac{2}{\sqrt{3}} M \sigma / d, \quad (8)$$

and for  $\varphi = 2$

$$\dot{\varepsilon}_{GBS} = M \sigma^2 / d. \quad (9)$$

If, on the other hand,  $M_a \neq M_b \neq M_c$  because boundary viscosity varies with grain orientation, the creep rate must be determined numerically by minimizing the work rate of the applied stress in achieving a given strain, say  $\dot{W}$ . Assuming normal grain boundary stresses are relaxed and that work is primarily spent in sliding,  $\dot{W} = \dot{x}_a T_a + \dot{x}_b T_b + \dot{x}_c T_c$ , then

$$\dot{W} \propto \sum_{\alpha} M_{\alpha}^{-1/\varphi} |\dot{S}_{\alpha} - \dot{\omega} \sqrt{3} d/2|^{(1+\varphi)/\varphi}.$$

where  $\alpha = a, b$  and  $c$  for the summation. Beeré (1978) optimizes the rate of rotation,  $\dot{\omega}$ , by minimizing  $\partial W / \partial \dot{\omega} = 0$  numerically, with  $\dot{\varepsilon} = constant$ ,  $d = constant$ , and  $\dot{S}_{\alpha} = constant$ .

When boundary viscosities vary by an order of magnitude,  $\dot{\omega}_{max} = 0.6\dot{\varepsilon}$ , and the maximum

angular variation of the array,  $\theta_{\max}$ , is never much greater than  $30^\circ$ .

Grain rotations are actually observed during creep, Figure 25.

Grain boundary sliding in "pure" materials is *anisotropic*: In general

$$v_{GBS}^i \equiv M_j^i \mathcal{T}^j,$$



where  $v_{GBS}^i$  denotes the components of the grain boundary sliding velocity  $v_{GBS}$ ,  $M_j^i$  denotes components of the *grain boundary mobility tensor*, and  $\mathcal{T}^j \equiv g_{kp} \sigma^{jk} n^p$  are components of the traction on a boundary with normal (unit) vector  $n$ ,  $\sigma^{jk}$  denoting components of the stress tensor (Raj and Ashby 1972). For "pure" materials  $\mathbf{M}$  is symmetric,  $M_j^i = M_i^j$ ; but if grain boundaries are influenced by second phase particles, subboundaries or dislocations, then additional relationships between the components of  $\mathbf{M}$  may develop. A random dispersion of (equiaxed) second phase particles produces "dimpled" grain boundaries, and in this case  $\mathbf{M}$  is isotropic, *i.e.* the number of components can be reduced to one,  $\mathbf{M} \equiv M_1^1 = M_2^2 = M_3^3$ . Then all grain boundaries slide at the same rate. This is assumed in Section 5.

Finally, for  $T > 0.7T_m$ , and for small shear stresses,  $\tau/G < 10^{-4}$ ,  $G$  denoting the shear modulus, Raj and Ashby (1972) found that grain boundary sliding in 99.999% silver containing hard, inert  $\text{SiO}_2$  and  $\text{Al}_2\text{O}_3$  particles was Newtonian viscous,  $\mu = 1$ , as in equation (8). Langdon (1970) on the other hand develops grain boundary sliding as a creep mechanism accommodated by grain boundary dislocation climb. He obtains the strain rate given by equation (9) with  $M$  proportional to the bulk diffusivity  $D_v$ .

## §4. Moving Unit Cells—Plasticity

At low temperatures and relatively high stresses metals deform plastically when dislocations *glide* across slip planes. For higher temperatures and lower stresses *dislocation climb* occurs: an edge dislocation line moves up or down, normal to the slip plane, via steps, or *jogs* in the core (Nabarro 1967, Hirth and Lothe 1982).

Dislocations experience a "*thermodynamic force*",

$${}^b\mathbf{F} \equiv F_m \mathbf{a}^m \equiv (\partial W / \partial x^m) \mathbf{a}^m, F_m \equiv -\partial G / \partial x^m = \partial W / \partial x^m,$$

where  $W$  is the *work* done by the applied stress in moving a dislocation over the distance represented by  $x^m$ , and  $G$  is the *free energy* of the system (Hirth, Hoagland and Popelar 1984). This "force" acts on the atomic configuration separating the slipped from the unslipped part of the crystal; it is not a force transmitted to atoms via the stress acting on the crystal surface. Figure 26 illustrates the "thermodynamic nature" of a "force" acting on an array of dislocations. The units of  ${}^b\mathbf{F}$  are  $[{}^b\mathbf{F}] = (\text{energy/atom})/\text{length} = \text{force/atom: } [W] = [G] = [F_m] = \text{energy/atom}, [\mathbf{a}^m] = [\mathbf{a}_m]^{-1} = \text{distance}^{-1}$ , and  $[x^m] = 1$ .

This "force" is determined as follows: The *Cauchy stress tensor*<sup>[42]</sup> is  $\sigma \equiv \sigma^{mn} \mathbf{a}_m \otimes \mathbf{a}_n$ ;  $\mathcal{T}(\mathbf{n}) \equiv \sigma \bullet \mathbf{n}$  is a *traction vector* with components  $\mathcal{T}^m = [\sigma \bullet \mathbf{n}]^m \equiv g_{np} \sigma^{mn} n^p$  where  $\mathbf{n}$  is a unit vector;  $\mathcal{T}^m$  is the force per unit (of deformed) area exerted on a surface

[42]: The stress tensor is symmetric, therefore its physical components are  $\sigma^{(mn)} \equiv (g_{mm}/g_{nn})\sigma^m_n$  (no sum), where  $\sigma^m_n \equiv \sigma^{mp} g_{pn}$  (Malvern 1969). Thus,  $[\sigma] = [\sigma^{mn} \mathbf{a}_m \otimes \mathbf{a}_n] = [\sigma^{(mn)}] = [\sigma^{mp} g_{pn}] = \text{pressure} \Rightarrow [\sigma^{mn}] = \text{force/area}^2$ , since  $[g_{mn}] = [\mathbf{a}_m \bullet \mathbf{a}_n] = \text{area}$ .

element with normal  $\mathbf{n}$  (Marsden and Hughes 1983). The stress<sup>[43]</sup>  $\sigma$  does work

$$W = \int_A \mathbf{b} \cdot \sigma \cdot d^2\mathbf{A} = \oint_L b_F$$

in creating the loop with area  $A$  and circumference  $L$  (Hirth and Lothe 1982). Here,  $d^2\mathbf{A}$  is a "differential" portion of the area  $A$ , which has a unit normal vector  $\mathbf{n}$ . This object is defined so that if  $\mathbf{v}$  is any vector then (Marsden and Hughes 1983)

$$\begin{aligned} \mathbf{v} \lrcorner \epsilon &\equiv \tfrac{1}{2} v^m \epsilon_{mpq} \vec{dx}^p \wedge \vec{dx}^q \equiv (\mathbf{v} \cdot \mathbf{n}) d^2\mathbf{A}, \\ &\equiv v^m \epsilon_{m|pq} \vec{dx}^p \wedge \vec{dx}^q, \end{aligned}$$

where the interior product ( $\lrcorner$ ) of  $p$ -form  $\omega$  and vector  $\mathbf{v}$  is the  $(p - 1)$ -form

$$\mathbf{v} \lrcorner \omega \equiv \frac{1}{(1-p)} v^m \omega_{mn_2\dots n_p} \vec{dx}^{n_2} \wedge \dots \wedge \vec{dx}^{n_p},$$

and of course  $\epsilon$  is a 3-form. Therefore,

[43]: Here,  $\sigma$  is the stress in the crystal, excluding the contribution from the self-stress of the dislocation loop.

[44]: Components of  $d^2\mathbf{A}$ ,  $[d^2\mathbf{A}]_m$ , are (Misner *et al.* 1973)

$$[d^2\mathbf{A}]_m \equiv \tfrac{1}{2} \epsilon_{mpq} \vec{dx}^p \wedge \vec{dx}^q \equiv \epsilon_{m|pq} \vec{dx}^p \wedge \vec{dx}^q.$$

$$\sigma \bullet d^2 A = a_m \otimes (\sigma^{mn} \epsilon_{n|pq} a^p \wedge a^q). [45]$$

By Stokes' theorem  $\oint_L b^F = \int_A \vec{d}^b F$ , so  $\vec{d}^b F = b \bullet \sigma \bullet d^2 A$ . Since  $b \bullet a_m = b^k a_k \bullet a_m = b^k g_{km}$

$$\vec{d}^b F = b \bullet \sigma \bullet d^2 A = b^k g_{km} \sigma^{mn} \epsilon_{n|pq} a^p \wedge a^q.$$

The quantity  $\vec{d}^b F$  is

$$\begin{aligned} \vec{d}^b F &= \vec{d}(F_q a^q) \equiv \vec{d} F_q \wedge a^q + F_q \vec{d} a^q, \\ &= (\partial F_q / \partial x^p) a^p \wedge a^q + F_q \vec{d} a^q, \\ &= (\partial F_q / \partial x^p) a^p \wedge a^q + \frac{1}{2} F_m T^m_{pq} a^p \wedge a^q, \end{aligned}$$

since  $\vec{d} a^q = \frac{1}{2} T^q_{kl} a^k \wedge a^l$ . Thus, dropping ' $\wedge a^q$ ' from both sides of  $\vec{d}^b F = b \bullet \sigma \bullet d^2 A$  gives

$$b_m \sigma^{mn} \epsilon_{n|pq} a^p = (\partial F_q / \partial x^p + F_m T^m_{pq}) a^p = -[\partial^2 G / \partial x^p \partial x^q + (\partial G / \partial x^m) T^m_{pq}] a^p \equiv \tilde{F}_q,$$

a different version of the *Peach-Koehler "force"* (1950)  $\tilde{F}_q$ . Inserting a unit vector  $\xi = \xi^p a_p$  tangent to the dislocation line into  $\tilde{F}_q(\dots)$  gives  $\tilde{F}_q \equiv \tilde{F}_q(\xi) \equiv \langle \tilde{F}_q, \xi \rangle$  for

[45]: The units of this object do not meet expectations: The area  $A$  can be defined

with two appropriately chosen vectors  $u, v$  as  $A = u \wedge v$ ,  $[A] = area$ , so that if

$$\sigma^{mn} = constant, \int_A \sigma \bullet d^2 A = a_m \otimes \int_{u \wedge v} \sigma^{mn} \epsilon_{n|pq} a^p \wedge a^q = a_m \sigma^{mn} \epsilon_{n|pq} \langle a^p \wedge a^q, u \wedge v \rangle =$$

$$a_m \sigma^{mn} \epsilon_{n|pq} \langle a^p \wedge a^q, a_r \wedge a_s \rangle u^r v^s = a_m \sigma^{mn} \epsilon_{n|pq} \delta^{pq}_{rs} u^r v^s = a_m \sigma^{mn} u^r v^s \epsilon_{n|pq} (\delta^p_r \delta^q_s - \delta^p_s \delta^q_r) =$$

$$a_m \sigma^{mn} u^r v^s (\epsilon_{n|rs} - \epsilon_{n|sr}) = a_m \sigma^{mn} \epsilon_{nrs} u^r v^s. \text{ The units of } a_m \sigma^{mn} \epsilon_{nrs} u^r v^s \text{ are}$$

*length*  $\times$  *force/area*<sup>2</sup>  $\times$  *volume*  $\times$  1  $\times$  1 = *force*, as expected.

$$\tilde{F}_q = b_m \epsilon_{qnp} \sigma^{mn} \xi^p = [\mathbf{b} \cdot \boldsymbol{\sigma} \times \boldsymbol{\xi}]_q.$$

Here,  $[F/L]_a \equiv [\mathbf{b} \cdot \boldsymbol{\sigma} \times \boldsymbol{\xi}]_a = e_{abc} b_d \sigma_{db} \xi_c$  is the usual citation of this "force" (Hirth and Lothe 1982), measured in the  $x^a$  reference frame, and its units are *force/length*. See Figure 27 for an illustration. The units of  $\tilde{F}_q$  are, on the other hand,  $[\tilde{F}_q] = [\tilde{F}_q] = \text{force/atom}$ :  $[b_m] = \text{area}$  since  $b_m = g_{mn} b^n$ ,  $[g_{mn}] = \text{area}$  and  $[b^n] = 1$ .

Figure 28 shows the two types of plastic deformation for a BCC crystal that are discussed here: glide and climb. *Dislocation glide* produces *slip* and results when the dislocation moves in the *slip plane*, which is the plane containing the dislocation line and the Burgers vector. *Dislocation climb* results when the dislocation moves perpendicular to the slip plane. Note for the case of dislocation glide that the dislocation axis translates one Burgers vector at a time by at most the simultaneous motion of all atoms in the dislocation core. Four of the forty-four atoms shown in Figure 28 are at the dislocation core. Thus, the indicated plastic shear of  $\gamma = 2\varepsilon = 1/6$  results from the simultaneous motion of at most about 1/10 of the atoms in the crystal. Therefore, as is well known, **plastic deformation of a crystal by dislocation motion is an inhomogeneous process**.

Figure 29 elucidates the difference between elastic and plastic deformations in a lattice with *sixfold* symmetry.

**Nearest neighbors remain nearest neighbors for an elastic deformation  
while plastic deformation results in atoms switching neighbors.**



The metric tensor  $\mathbf{g} = g_{mn} \vec{dx}^m \otimes \vec{dx}^n$  is dragged by a plastic deformation (Marcinkowski 1979), *i.e.* it is unaffected. "A transformation that preserves the metric is called an *isometry*. Such a transformation maps a figure into an image that is the same metric size and shape" (Burke 1985). Consider the case of crystal slip via dislocation glide and let  $\mathbf{u}$  denote the *plastic displacement field*. Since elastic displacements have already been accounted for in the metric  $\mathbf{g}$ ,  $\mathbf{u}$  can denote the plastic displacement field instead of  $\mathbf{\tilde{u}}$ . The magnitude of  $\mathbf{u}$ ,  $u$ , is large enough to move an atom from its original position  $\rho$  to the next available position with the same crystallographic symmetry,  $\rho + \mathbf{b}$ , where  $\mathbf{u} \equiv \mathbf{b}$ . For BCC crystals,  $\mathbf{b} = \frac{1}{2}a\langle 111 \rangle$ , and for FCC crystals  $\mathbf{b} = \frac{1}{2}a\langle 110 \rangle$ , where  $a$  is the lattice parameter of the respective conventional unit cell,  $a_x \approx a_y \approx a_z \equiv a$ , and  $\langle 111 \rangle$  and  $\langle 110 \rangle$  are families of crystallographic directions referred to these conventional unit cells. The plastic displacements  $\mathbf{u} \equiv \mathbf{b}$  occur on the slip planes. Atoms in the dislocation core on opposite sides of the slip plane suffer relative displacements of  $\mathbf{u} \equiv \mathbf{b}$  when the defect *glides* a distance  $\mathbf{b}$ . If there are many active, parallel slip planes in the lattice, then a shear stress deforms it like a pack of cards; this is called *laminar flow*. The slip planes are otherwise unaffected by this process.

The "Killing vector" is used in differential geometry to describe "symmetry" (Misner *et al.* 1973). "A *symmetry* is a transformation that leaves the structure essentially unchanged. Some symmetries, such as reflections in a plane, are discrete. Others, such as translations and rotations, form continuous sets. *Continuous symmetries* are best approached via their infinitesimal generators, and these are represented by vectors fields. ... A vector field that generates an *infinitesimal isometry* is called a *Killing vector*" (Burke 1985). Here the vector

field is  $\mathbf{u}$ . A *Killing vector field* ( $\mathbf{u}$ ) satisfies *Killing's equation* (Burke 1985),  $\mathbf{L}_u \mathbf{g} = \mathbf{0}$ , and preserves the unit density  $*1 = \epsilon = \vec{d}x^m \wedge \vec{d}x^n \wedge \vec{d}x^p$ . In addition,  $\mathbf{L}_u \mathbf{T}^m = \mathbf{0}$ , where  $\mathbf{T}^m \equiv \frac{1}{2} T_{pn}^m \mathbf{a}^n \wedge \mathbf{a}^p$  (Dereli and Vercin 1987).

Killing's equation  $\mathbf{L}_u \mathbf{g} = \mathbf{0}$  says that  $\mathbf{g}$  is *Lie transported*, or dragged along the vector field  $\mathbf{u}$ . Any solution to Killing's equation is a linear combination of translations  $\mathbf{u}_{\mathcal{T}}$  and rotations  $\mathbf{u}_{\mathcal{R}}$ ; the solution is  $\mathbf{u} = \text{const.}_{\mathcal{T}} \mathbf{u}_{\mathcal{T}} + \text{const.}_{\mathcal{R}} \mathbf{u}_{\mathcal{R}}$  (Burke 1985, Wasserman 1992). For primitive unit cells:

$$\mathbf{u}_{\mathcal{T}} \equiv \mathbb{I}_x \mathbf{a}_x + \mathbb{I}_y \mathbf{a}_y + \mathbb{I}_z \mathbf{a}_z \equiv \vec{\mathbb{I}} \cdot \vec{\mathbf{a}},$$

and

$$\mathbf{u}_{\mathcal{R}} \equiv \mathbb{I}_x(z\mathbf{a}_y - y\mathbf{a}_z) + \mathbb{I}_y(x\mathbf{a}_z - z\mathbf{a}_x) + \mathbb{I}_z(y\mathbf{a}_x - x\mathbf{a}_y) \equiv \begin{vmatrix} \mathbb{I}_x & \mathbb{I}_y & \mathbb{I}_z \\ \mathbf{a}_x & \mathbf{a}_y & \mathbf{a}_z \\ x & y & z \end{vmatrix} \equiv \vec{\mathbb{I}} \cdot \vec{\mathbf{a}} \times \vec{\mathbf{c}}.$$

Here:  $\mathbf{a}_n \equiv (\partial/\partial x^n) \equiv \vec{\partial}_n$ , and  $\vec{\mathbf{a}} \equiv (\mathbf{a}_x, \mathbf{a}_y, \mathbf{a}_z)$ ;  $\mathbb{I}_n$  are integers, and  $\vec{\mathbb{I}} \equiv (\mathbb{I}_x, \mathbb{I}_y, \mathbb{I}_z)$ ; and  $\mathbf{a}_n \equiv \mathbf{b}_n$  are the lattice displacements which preserve the crystal symmetry (*e.g.* the Burgers vectors). The vectors  $\vec{\mathbf{a}}$  and  $\vec{\mathbb{I}}$  belong to a six-dimensional *configuration manifold* with unit vectors (not named) as a basis: there are three rotational degrees of freedom and three translational degrees of freedom (Dereli and Vercin 1987), not all of which may be operative in any given lattice structure. The defects responsible for translations ( $\mathbf{u}_{\mathcal{T}}$ ) are dislocations, while those responsible for rotations ( $\mathbf{u}_{\mathcal{R}}$ ) are disclinations (Kröner and Anthony 1975). For laminar flow from dislocation slip on a single set of glide planes,  $\mathbf{u}_{\mathcal{T}} \equiv \mathbb{I}_x \mathbf{a}_x$ , for example.

Dereli and Vercin (1987) use Killing's equation for disclinations in a "gauge model" of amorphous solids. The applicability of Killing's equation to dislocation motion appears to be unrecognized, but it is suggestive of Weingarten's theorem,<sup>[46]</sup> Bilby *et al.*'s (1958) analysis of single glide and plane strain, some material discussed by Venkataraman and Sahoo (1986) and Kröner (1959/60), and the "gauge theories" of defect dynamics, *e.g.* Golebiewska-Lasota and Edelen (1979).

*Plastic deformation* can be simply modelled as many dislocations gliding on many slip planes, *e.g.* Taylor (1934), as shown by Figure 30.

Edelen (1979) uses 1-forms  $\mathbf{J}^m$  and  $\mathbf{S}^m$  for the dislocation and disclination currents, respectively. The *dislocation current 1-forms* are  $\mathbf{J}^n \equiv J_{M^n} \vec{d}X^M$ , and<sup>[47]</sup> the *disclination current 2-forms* are  $\mathbf{S}^n \equiv \frac{1}{2} S^{Mn} \epsilon_{MNP} \vec{d}X^N \wedge \vec{d}X^P$ , such that the temporal dependency of  $\tilde{\mathbf{p}}^n \equiv \frac{1}{2} \rho^{Mn} \epsilon_{MNP} \vec{d}X^N \wedge \vec{d}X^P$  is

$$\partial \tilde{\mathbf{p}}^n / \partial t = -\vec{d}\mathbf{J}^n - \mathbf{S}^n,$$

and

$$\partial b^n / \partial t = -\int_C \mathbf{J}^n, \quad \partial \ell^n / \partial t = -\int_V \mathbf{S}^n,$$

where  $b^n = -\int_V \tilde{\mathbf{p}}^n$ , and  $\ell^n = -\int_V \Theta^n = -\int_V \vec{d}\tilde{\mathbf{p}}^n$ , are the Burgers vectors for dislocations and disclinations, respectively. Here,  $C$  is the closed boundary of the two dimensional

[46]: See the note following the caption for Figure 14.

[47]: Kosevich (1979) refers to the components of  $\mathbf{J}^m$ ,  $J_{M^m}$ , as the *dislocation flux density*.

surface  $\partial \mathbf{V}$  around the volume  $\mathbf{V}$  in the deformed lattice through which Burgers vectors  $b^n$  pass through at the "rate"  $\partial b^n / \partial t$ , and similarly for the disclinations;  $\Theta^n \equiv \Theta^n \epsilon \equiv \vec{d} \tilde{\rho}^n \equiv (\partial \rho^{Mn} / \partial X^M) \vec{d}X^M \wedge \vec{d}X^N \wedge \vec{d}X^P$  is the disclination density 3-form,  $\Theta^n \equiv \partial \rho^{Mn} / \partial X^M$ . The dislocation density tensor  $\rho = \rho^{Mn} \mathbf{A}_M \otimes \mathbf{a}_n$ , where  $\rho^{Mn} = \epsilon^{MPQ} \partial_{[P} \gamma_{Q]n} = \frac{1}{2} \epsilon^{MPQ} T^n_{PQ}$ , can be reexpressed as the 2-forms  $\tilde{\rho}^n$ :

$$\tilde{\rho}^n \equiv \frac{1}{2} \rho^{Mn} \epsilon_{MNP} \vec{d}X^N \wedge \vec{d}X^P \equiv \frac{1}{2} T^n_{NP} \vec{d}X^N \wedge \vec{d}X^P \equiv -T^n,$$

$$\tilde{\rho}^n_{NP} \equiv \epsilon_{MNP} \rho^{Mn} \equiv T^n_{NP}.$$

Dislocations move by climb and glide in the BCC "dual" lattice to the cellular array that models a polycrystalline microstructure, causing the cellular array to flow. Disclination motion in this lattice results in grain rotations, which are known to occur during superplastic deformation since preferred crystallographic orientation (texture) is often destroyed (Ashby and Verrall 1973); but disclination motion is not developed here, see Edelen (1979) for further details. The following sub-section is a simplistic overview of Edelen's (1979) work, which is summarized in the next box.<sup>[48]</sup> Afterwards the tensile specimen is "geometrized" and the Orowan equation written. The section closes with a review of constitutive relationships for plastic deformation.

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[48]: See Nabarro (1967) and Kosevich (1979) for a "conventional" tensor analysis approach to this material.

### Summary of Edelen's (1979) Field Equations for Dislocation Dynamics

$$\begin{aligned}
 x^m &= \chi^m(X^M, t), & v^m &\equiv \partial \chi^m / \partial t; \\
 \tilde{\gamma}^m &\equiv {}_{in}\tilde{\gamma}^m + {}_{ex}\tilde{\gamma}^m = \gamma_M^m \vec{d}X^M + \vec{d}\chi^m = \gamma_M^m \vec{d}X^M + (\partial \chi^m / \partial X^M) \vec{d}X^M; \\
 \tilde{\rho}^m &= \frac{1}{2} \rho^{Mm} \epsilon_{MNP} \vec{d}X^N \wedge \vec{d}X^P, & \rho^{Mm} &= \epsilon^{MPQ} \partial_P \gamma_Q^m, \quad T^m_{NP} = \epsilon_{MNP} \rho^{Mm}; \\
 \tilde{\rho}^m &= \vec{d}\tilde{\gamma}^m = \partial_N \gamma_M^m \vec{d}X^N \wedge \vec{d}X^M + \mathbf{0} = \frac{1}{2} (\partial_N \gamma_M^m - \partial_M \gamma_N^m) \vec{d}X^N \wedge \vec{d}X^M; \\
 &&&= \frac{1}{2} T^m_{NM} \vec{d}X^N \wedge \vec{d}X^M \equiv -\mathbf{T}^m; \\
 \tilde{\rho}^m &= \vec{d}\tilde{\gamma}^m \Rightarrow \vec{d}\tilde{\rho}^m = \mathbf{0} \text{ since } \vec{d}^2\tilde{\gamma}^m = \mathbf{0}; \\
 \partial \tilde{\gamma}^m / \partial t + \mathbf{J}^m &= \vec{d}v^m, & \mathbf{J}^m &= J_M^m \vec{d}X^M; \\
 \partial \tilde{\rho}^m / \partial t &= -\vec{d}\mathbf{J}^m \equiv -(\partial J_M^m / \partial X^N) \vec{d}X^N \wedge \vec{d}X^M \equiv -\partial_{[N} J_{M]}^m \vec{d}X^N \wedge \vec{d}X^M.
 \end{aligned}$$

<u>Term</u>	<u>Meaning</u>
$x^m = \chi^m(X^M, t)$	Current configuration of body, $x^m$ , is a function, $\chi^m$ , of the reference configuration $X^M$ and time $t$ .
$v^m$	Velocity relative to reference configuration.
$\tilde{\gamma}^m$	The distortion 1-form is the sum of an inexact (internal) term, ${}_{in}\tilde{\gamma}^m \equiv \gamma_M^m \vec{d}X^M$ , and an exact (external) term ${}_{ex}\tilde{\gamma}^m \equiv \partial_M \chi^m \vec{d}X^M$ .
$\tilde{\rho}^m$	Dislocation density 2-form ( $\tilde{\rho}^m_{NP} \equiv \epsilon_{MNP} \rho^{Mm} \equiv T^m_{NP}$ ).
$\rho^{Mm}$	Dislocation density tensor $\rho \equiv \rho^{Mn} \mathbf{A}_M \otimes \mathbf{a}_n$ .
$T^m_{NM}$	Torsion tensor: $T^m_{NM} \equiv \mathbf{T}(\mathbf{a}^m, \mathbf{A}_M, \mathbf{A}_N)$ .
$\mathbf{J}^m$	Dislocation current 1-forms: $\partial b^n / \partial t = -\int_C \mathbf{J}^n$ .

#### 4.1. The Strain Rate

Let  $\chi^m$  be functions which give the current geometric configuration of the boundary,  $\mathbf{S}$ , of a complexion of corpuscles which deform together compatibly from a single mechanism. The boundary  $\mathbf{S}$  has coordinates  $x^m$  that are functions of the reference coordinates  $X^M$  and time  $t$ :

$$\begin{aligned} x^m &= \chi^m(X^M, t), \quad X^M = [\chi^m]^{-1}(x^m, t); \\ \mathbf{a}_m &\equiv \vec{d}\chi^m \equiv (\partial\chi^m/\partial X^M)\vec{d}X^M \equiv L^m_M \vec{d}X^M \equiv L^m_M \mathbf{A}^M; \\ \mathbf{a}_m &\equiv \partial/\partial x^m \equiv (\partial X^M/\partial x^m)\partial/\partial X^M = (\partial[\chi^m]^{-1}/\partial x^m)\partial/\partial X^M \equiv L_m^M \partial/\partial X^M \equiv L_m^M \mathbf{A}_M; \\ L^m_M L_m^N &= (\partial x^m/\partial X^M)(\partial X^N/\partial x^m) = \partial X^N/\partial X^M = \delta_M^N. \end{aligned}$$

Here of course, the  $x^m$  coordinates, and tangent  $\mathbf{a}_m$  and cotangent  $\mathbf{a}^m \equiv \vec{d}x^m \equiv \vec{d}\chi^m$  basis vectors are for the boundary  $\mathbf{S}$ . Dislocations inside  $\mathbf{S}$  are responsible for the *non-integrable* or *internal response* of the lattice while the 1-forms  $\vec{d}\chi^m \equiv (\partial\chi^m/\partial X^M)\vec{d}X^M$  give the *integrable* or *external response* of the specimen: *i.e.*  $L^m_M \equiv \partial\chi^m/\partial X^M$  are the *externally measurable deformation gradients* of the specimen.<sup>[49]</sup> The coordinate mesh for the shape strain is coarser than that for the lattice (Christian 1965). Since the functions  $\chi^m$  which give the coordinates  $x^m$  of the simply-connected region  $\mathbf{S}$  are everywhere smooth and differentiable,  $\vec{d}^2\chi^m \equiv 0$ . Therefore adding  $\vec{d}\chi^m$  to  $\tilde{\gamma}^m \equiv \gamma_M^m \vec{d}X^M$  does not affect exterior differentiation of  $\tilde{\gamma}^m$ , because the external distortions are conservative, or exact. So "new"  $\tilde{\gamma}^m$  can be defined with the

[49]: The lattice planes containing the Burgers vector and dislocation axis do not move relative to the reference configuration until a dislocation reaches a free surface.

"gauge transformation"

$$\begin{aligned}\tilde{\gamma}^m &\equiv {}_{in}\tilde{\gamma}^m + {}_{ex}\tilde{\gamma}^m; \\ {}_{in}\tilde{\gamma}^m &\equiv \gamma_M^m \vec{d}X^M, \text{ and } {}_{ex}\tilde{\gamma}^m \equiv (\partial\chi^m/\partial X^M) \vec{d}X^M \equiv L^m_M \vec{d}X^M; \\ \vec{d}\tilde{\gamma}^m &= \vec{d}{}_{in}\tilde{\gamma}^m + \mathbf{0}.\end{aligned}$$

Measures of strain derived from  $\partial\chi^m/\partial X^M$  represent *total geometric strains* (elastic + plastic), which Bilby (1960) calls the ***shape strain***:

$$\begin{aligned}\mathcal{E}(\dots, \dots) &= \mathcal{E}_{MN} \vec{d}X^M \otimes \vec{d}X^N, \\ \mathcal{E}_{MN} &= \frac{1}{2} [(\partial_M \chi^m) \delta_{mn} (\partial_N \chi^n) - \delta_{MN}] = \frac{1}{2} (\delta_{mn} L^m_M L^n_N - \delta_{MN}) \equiv \varepsilon_{MN} + \mathcal{E}_{MN}.\end{aligned}$$

The strain rate  $\dot{\mathcal{E}} = \dot{\mathcal{E}}_{MN} \vec{d}X^M \otimes \vec{d}X^N$  has components  $\dot{\mathcal{E}}_{MN} \equiv \partial \mathcal{E}_{MN} / \partial t \equiv \dot{\varepsilon}_{MN} + \dot{\mathcal{E}}_{MN}$ :

$$\dot{\mathcal{E}}_{MN} = \frac{1}{2} \partial [(\partial_M \chi^m) \delta_{mn} (\partial_N \chi^n) - \delta_{MN}] / \partial t = \frac{1}{2} [(\partial_M v^m) \delta_{mn} L^n_N + L^m_M \delta_{mn} (\partial_N v^n)];$$

or, with respect to the  $x^m$  coordinates:

$$\begin{aligned}\dot{\mathcal{E}}_{pq} &= L_p^M L_q^N \dot{\mathcal{E}}_{MN} = \frac{1}{2} L_p^M L_q^N [(\partial_M v^m) \delta_{mn} L^n_N + L^m_M \delta_{mn} (\partial_N v^n)], \\ &= \frac{1}{2} [(L_p^M \partial_M v^m) \delta_{mn} L_q^N L^n_N + L_p^M L^m_M \delta_{mn} (L_q^N \partial_N v^n)], \\ &= \frac{1}{2} [(\partial_p v^m) \delta_{mn} \delta_q^n + \delta_p^m \delta_{mn} (\partial_q v^n)], \quad (\partial_p = L_p^M \partial_M, \quad L_q^N L^n_N = \delta_q^n) \\ &= \frac{1}{2} [\delta_{mq} \partial_p v^m + \delta_{pn} \partial_q v^n]. \quad (\text{Cited by Kosevich (1979).})\end{aligned}$$

Here,  $v^m$  denote the *total velocity 0-forms* ( $v^x, v^y, v^z$ ):  $v^m \equiv \partial \chi^m / \partial t$ . The velocity with which  $\mathbf{S}$  moves relative to the reference configuration is  $\mathbf{v} = v^m \mathbf{a}_m$ .

In the absence of disclinations

$$\begin{aligned}\partial \tilde{\mathbf{p}}^m / \partial t &= -\vec{\mathbf{d}} \mathbf{J}^m = -(\partial J_{N^m} / \partial X^P) \vec{\mathbf{d}} X^P \wedge \vec{\mathbf{d}} X^N, \\ &= -\partial_{[P} J_{N]m} \vec{\mathbf{d}} X^P \wedge \vec{\mathbf{d}} X^N,\end{aligned}$$

where  $\partial_{[P} J_{N]m} \equiv \frac{1}{2} (\partial J_{N^m} / \partial X^P - \partial J_{P^m} / \partial X^N)$ ; with  $\tilde{\mathbf{p}}^m = \vec{\mathbf{d}} \tilde{\mathbf{y}}^m = \partial_{[P} \gamma_{N]m} \vec{\mathbf{d}} X^P \wedge \vec{\mathbf{d}} X^N = \frac{1}{2} T^m_{PN} \vec{\mathbf{d}} X^P \wedge \vec{\mathbf{d}} X^N$ , this becomes

$$(\frac{1}{2} \partial T^m_{PN} / \partial t + \partial_{[P} J_{N]m}) \vec{\mathbf{d}} X^P \wedge \vec{\mathbf{d}} X^N = \mathbf{0}.$$

Components for this relationship are

$$\partial T^m_{PN} / \partial t + 2 \partial_{[P} J_{N]m} = 0;$$

and its dual is the 1-form  $\frac{1}{2} \epsilon_{QRS} G^{RP} G^{SN} [\partial T^m_{PN} / \partial t + (\partial_P J_{N^m} - \partial_N J_{P^m})] \vec{\mathbf{d}} X^Q$ , which can be converted to the following vector, for comparison with Kosevich (1979):

$$\begin{aligned}*(\frac{1}{2} \partial T^m_{PN} / \partial t + \partial_{[P} J_{N]m}) \vec{\mathbf{d}} X^P \wedge \vec{\mathbf{d}} X^N &= \frac{1}{2} \epsilon_{QRS} G^{RP} G^{SN} [\partial T^m_{PN} / \partial t + (\partial_P J_{N^m} - \partial_N J_{P^m})] \vec{\mathbf{d}} X^Q, \\ &= \frac{1}{2} \epsilon_{QRS} G^{RP} G^{SN} [\partial T^m_{PN} / \partial t + (\partial_P J_{N^m} - \partial_N J_{P^m})] G^{QM} \mathbf{A}_M, \\ &= \frac{1}{2} \epsilon_{QRS} G^{QM} G^{RP} G^{SN} [\partial T^m_{PN} / \partial t + (\partial_P J_{N^m} - \partial_N J_{P^m})] \mathbf{A}_M, \\ &= \frac{1}{2} \epsilon^{MPN} [\partial T^m_{PN} / \partial t + (\partial_P J_{N^m} - \partial_N J_{P^m})] \mathbf{A}_M, \\ (\epsilon^{MPN} &= \epsilon_{QRS} G^{QM} G^{RP} G^{SN}) \\ &= [\partial \rho^{Mm} / \partial t + \epsilon^{MPN} \partial_P J_{N^m}] \mathbf{A}_M. \quad (\rho^{Mm} = \frac{1}{2} \epsilon^{MPN} T^m_{PN}).\end{aligned}$$

Thus,

$$\partial \rho^{\text{Mm}} / \partial t + \epsilon^{\text{MPN}} \partial_p J_{N^m} = 0$$

is the differential version of the law for the *conservation of the Burgers vector* (Kosevich 1979).

A "trivial" compatibility statement also follows from the relationship  $\partial \tilde{\mathbf{p}}^m / \partial t = -\vec{\mathbf{d}} \mathbf{J}^m$ :

$$\begin{aligned}\partial \tilde{\mathbf{p}}^m / \partial t + \vec{\mathbf{d}} \mathbf{J}^m &= \partial (\vec{\mathbf{d}} \tilde{\mathbf{Y}}^m) / \partial t + \vec{\mathbf{d}} \mathbf{J}^m = \mathbf{0} \Rightarrow \\ \vec{\mathbf{d}} (\partial \tilde{\mathbf{Y}}^m / \partial t + \mathbf{J}^m) &= \vec{\mathbf{d}} (\partial_{in} \tilde{\mathbf{Y}}^m / \partial t + \partial_{ex} \tilde{\mathbf{Y}}^m / \partial t + \mathbf{J}^m) = \mathbf{0}.\end{aligned}$$

If "well behaved" functions can be found such that their exterior derivatives are equal to  $\partial \tilde{\mathbf{Y}}^m / \partial t + \mathbf{J}^m$ , then  $\vec{\mathbf{d}} (\partial \tilde{\mathbf{Y}}^m / \partial t + \mathbf{J}^m) = \mathbf{0}$  will be an identity; these functions are just the  $v^m$ :

$$\begin{aligned}\partial \tilde{\mathbf{Y}}^m / \partial t + \mathbf{J}^m &\equiv \vec{\mathbf{d}} v^m \Rightarrow \vec{\mathbf{d}}^2 v^m = \vec{\mathbf{d}} (\partial \tilde{\mathbf{Y}}^m / \partial t + \mathbf{J}^m) = \mathbf{0}, \\ \vec{\mathbf{d}} v^m &= (\partial v^m / \partial X^M) \vec{\mathbf{d}} X^M = (\partial_M v^m) \vec{\mathbf{d}} X^M.\end{aligned}$$

Therefore

$$\partial \tilde{\mathbf{Y}}^m / \partial t + \mathbf{J}^m = \vec{\mathbf{d}} v^m \text{ or, } \partial_{in} \tilde{\mathbf{Y}}^m / \partial t + \partial_{ex} \tilde{\mathbf{Y}}^m / \partial t + \mathbf{J}^m = \vec{\mathbf{d}} v^m,$$

or

$$(\partial \gamma_{M^m} / \partial t) \vec{\mathbf{d}} X^M + [\partial (\partial_M \chi^m) / \partial t] \vec{\mathbf{d}} X^M + J_{M^m} \vec{\mathbf{d}} X^M = \partial_M v^m \vec{\mathbf{d}} X^M.$$

This is trivial because  $J_{M^m} = -\partial \gamma_{M^m} / \partial t$  and  $v^m \equiv \partial \chi^m / \partial t$ : the condition for the compatibility of the two expressions

$$(1) \quad \mathbf{p} = \rho^{Mm} \mathbf{A}_M \otimes \mathbf{a}_m \equiv \epsilon^{MPQ} \partial_{[P} \gamma_{Q]m} \mathbf{A}_M \otimes \mathbf{a}_n = \frac{1}{2} \epsilon^{MPQ} T^n_{\quad PQ} \mathbf{A}_M \otimes \mathbf{a}_n$$

and

$$(2) \quad \partial \tilde{\gamma}^m / \partial t + \mathbf{J}^m = \tilde{\mathbf{d}} v^m$$

is that the relationships

$$(\frac{1}{2} \partial T^m_{\quad PN} / \partial t + \partial_{[P} J_{N]}^m) \tilde{\mathbf{d}} X^P \wedge \tilde{\mathbf{d}} X^N = \mathbf{0}$$

hold, or equivalently that their dual

$$[\partial \rho^{Mm} / \partial t + \epsilon^{MNP} \partial_P J_N^m] \mathbf{A}_M = \mathbf{0}$$

be satisfied (Kosevich 1979). This compatibility argument states that the internal response of dislocation motion,  $J_M^m = -\partial \gamma_M^m / \partial t$ , results in an external response (measurable strain rate) proportional to  $\partial_M v^m = \partial (\partial_M \chi^m) / \partial t$ . It is general practice to assume that the internal motion of defects gives rise to an equivalent, measurable total strain rate, as in for example, the development of the Orowan equation, the next topic.

## 4.2. The Orowan Equation

### 4.2.1. "Geometrization" of the Tensile Specimen

Let  $\mathbf{U}, \mathbf{V}, \mathbf{W}$  be vectors that define the boundary  $\mathbf{S}$  of a complexon of corpuscles which deform together compatibly from a single mechanism, Figure 31a. The volume inside  $\mathbf{S}$  is given by the trivector  $\vec{\mathbf{V}}$ :

$$\vec{\mathbf{V}} \equiv \mathbf{U} \wedge \mathbf{V} \wedge \mathbf{W} \equiv \gamma^{xyz} \mathbf{a}_x \wedge \mathbf{a}_y \wedge \mathbf{a}_z \equiv \frac{1}{3!} \begin{vmatrix} U^x & U^y & U^z \\ V^x & V^y & V^z \\ W^x & W^y & W^z \end{vmatrix} \mathbf{a}_x \wedge \mathbf{a}_y \wedge \mathbf{a}_z;$$

$\vec{\mathbf{V}}$  is a simple trivector because it is just a determinant of three vectors (Schouten 1989)

$$\gamma^{xyz} \equiv U^x(V^y W^z - W^y V^z) + U^y(V^z W^x - W^z V^x) + U^z(V^x W^y - W^x V^y) \equiv 3! U^{[x} V^y W^{z]}. \text{ [50]}$$

Now  $|\vec{\mathbf{V}}| = \text{volume}$  and  $\gamma^{xyz}$  is unit-less in the  $x^m$  coordinate system. The Levi-Cevita tensor can be written with the tangent basis vectors  $\mathbf{a}_q$  as  $\epsilon = \frac{1}{3!} e^{mnp} \mathbf{a}_m \wedge \mathbf{a}_n \wedge \mathbf{a}_p$  (Tonti 1976),  $e^{mnp}$  denoting contravariant components of the (unit-less) permutation tensor. Also,

$$\vec{\mathbf{V}} \equiv \gamma^{qrs} \mathbf{a}_q \wedge \mathbf{a}_r \wedge \mathbf{a}_s \equiv \frac{1}{3!} \gamma^{qrs} \mathbf{a}_q \wedge \mathbf{a}_r \wedge \mathbf{a}_s,$$

[50]: The permutation symbol,  $[]$ , on three indices means the following:

$$U^m V^n W^{p!} \equiv \frac{1}{3!} (U^m V^n W^p + U^n V^p W^m + U^p V^m W^n - U^m V^p W^n - U^n V^m W^p - U^p V^n W^m).$$

vertical bars again denoting summation over the restricted range  $q < r < s$ , and

$$\begin{aligned}
\vec{\mathbf{V}} \cdot \vec{\mathbf{V}} &\equiv U_{[m} V_{n} W_{p]} U^{[q} V^{r} W^{s]} \langle \mathbf{a}^m \wedge \mathbf{a}^n \wedge \mathbf{a}^p, \mathbf{a}_q \wedge \mathbf{a}_r \wedge \mathbf{a}_s \rangle, \\
&\equiv U_{[m} V_{n} W_{p]} U^{[q} V^{r} W^{s]} \delta^{mnp}_{qrs}, \\
&= U_{[m} V_{n} W_{p]} U^m V^n W^p; \text{ (Misner et al. 1973)} \\
&= U^2 V^2 W^2, \\
&\equiv \|\vec{\mathbf{V}}\|^2, \\
&\equiv \gamma^2. \text{ (Only for rectangular geometry.)}
\end{aligned}$$

For a "coordinate transformation" from the reference frame  $x^a$  to the deformed crystallographic coordinates  $x^m$ ,  $x^a \rightarrow x^m$ ,  $x^m = x^m(x^a)$ ,<sup>[51]</sup> trivectors "transform" like this (Schouten 1989):

$$\begin{aligned}
\gamma^{mnp} &= 3! U^{lm} V^n W^{pl} = 3! \lambda^m_a \lambda^n_b \lambda^p_c U^a V^b W^c, \\
&\equiv 3! |\partial x^m / \partial x^a| U^a V^b W^c, \\
&\equiv 3! \Omega^{-1} U^a V^b W^c \equiv \Omega^{-1} \gamma^{abc},
\end{aligned}$$

[51]: Recall for a "coordinate transformation"  $x^a \rightarrow x^m(x^a)$  that cotangent and tangent basis vectors "transform" like

$\vec{\mathbf{d}}x^m \equiv (\partial x^m / \partial x^a) \vec{\mathbf{d}}x^a \equiv \lambda^m_a \vec{\mathbf{d}}x^a$ ,  $\vec{\mathbf{d}}x^a = \lambda_m^a \vec{\mathbf{d}}x^a$ ;  $\mathbf{a}_m \equiv \lambda_m^a \mathbf{a}_a$ ,  $\mathbf{i}_a = \lambda^m_a \mathbf{a}_m$ ;  
 $\vec{\mathbf{d}}x^m \equiv \mathbf{a}^m$ ,  $\vec{\mathbf{d}}x^a \equiv \mathbf{i}^a$ ,  $\partial / \partial x^a \equiv \mathbf{i}_a$ ,  $\partial / \partial x^m \equiv \mathbf{a}_m$ ;  $\lambda_m^a \lambda^m_b = \delta^a_b$ . The  $x^a$  have units of distance while the  $x^m$  are dimensionless;  $\mathbf{i}_a$  and  $\mathbf{i}^a$  are dimensionless,  $[\vec{\mathbf{d}}x^m] = distance^{-1}$ ,  $[\mathbf{a}_m] = distance$ . Contravariant objects "transform" like  $v^m = \lambda^m_a v^a$  and  $v^a = \lambda_m^a v^m$ , and covariant objects "transform" like  $\omega_m = \lambda_m^a \omega_a$  and  $\omega_a = \lambda^m_a \omega_m$ .

where  $\Omega^{-1} \equiv |\partial x^m / \partial x^a|$ , vertical bars denoting determinant,  $\mathcal{V}^{abc} \equiv 3! U^a V^b W^c$  has dimensions of volume, and  $\mathcal{V}^{abc} = \Omega \mathcal{V}^{mnp}$ . The object  $\vec{\mathbf{V}} \equiv \mathbf{U} \wedge \mathbf{V} \wedge \mathbf{W}$  is invariant. I will not show the components, since the object has a single value because it is a *scalar density* (of "weight" —1) (Schouten 1989), writing instead  $\gamma(x^m)$  for  $\mathcal{V}^{mnp}$  and  $\gamma(x^a)$  for  $\mathcal{V}^{abc}$ .

Plastic deformation is a constant volume process and therefore  $\mathcal{V} = \text{constant}$ .

#### 4.2.2. "Geometrization" of the Slip System

Consider a crystallographic coordinate system based upon the primitive unit cell of the BCC lattice, Figure 31b (see also Figure 28). Burgers vectors are from the family of directions  $<111>$ , and slip planes are from the family of planes  $\{110\}$ . Let the Burgers vector be  $\mathbf{b} \equiv \mathbf{a}_x \equiv \frac{1}{2}a[1\bar{1}\bar{1}] \equiv a_x \mathbf{i}$ , where  $\mathbf{i} \equiv \mathbf{a}_x / \|\mathbf{a}_x\| = [1\bar{1}\bar{1}] / \sqrt{3}$ , and  $a_x \equiv \|\mathbf{a}_x\| \equiv (\mathbf{a}_x \cdot \mathbf{a}_x)^{1/2} = (\sqrt{3}/2)a$ . Here,  $a$  denotes the lattice parameter for the conventional unit cell in the elastically deformed condition; it must be an average of the lengths of the twelve sides of the conventional unit cell. The positive edge segment of the dislocation has an axis with unit vector  ${}^{\text{edge}}\xi$  along the crystallographic direction  $-[111]/\sqrt{3} \equiv -\mathbf{j}$ ; the right-hand screw segment has direction  ${}^{\text{screw}}\xi$  along  $[1\bar{1}\bar{1}]/\sqrt{3} \equiv \mathbf{i}$ ;  $\mathbf{a}_y \equiv \frac{1}{2}a[111] \equiv a_y \mathbf{j}$ , and therefore  $\mathbf{a}_z = \frac{1}{2}a[1\bar{1}1] \equiv a_z \mathbf{k}$  for a right-hand coordinate system,  $\mathbf{k} \equiv [1\bar{1}1]/\sqrt{3}$ . Dislocation glide induces slip through the relative motion of unit cells at edge segments of the dislocation core, in the  $\mathbf{b}$ -direction, and at the rate  $\mathbf{v} = v^x \mathbf{a}_x$ . The slip plane is proportional to  $\mathbf{b} \wedge \xi$ , and is therefore represented by the bivector

$$\vec{\mathbf{A}} \equiv A \mathbf{a}_x \wedge \mathbf{a}_y,$$

with the dimensions  $[\vec{\mathbf{A}}] = \text{area}$ ,  $A$  is unit-less when measured with the  $x^m$  coordinates.

Let the glide plane bisect the volume  $\vec{\mathbf{V}}$  into  $n$  volumes, where  $n = 2$  for Figure 31.

Then "tubes" (2-forms) of material

$$\tilde{\mathbf{A}} \equiv nA^{-1}\mathbf{a}^x \wedge \mathbf{a}^y$$

suffer relative translations over glide planes  $\vec{\mathbf{A}}$  at the rate  $\mathbf{v}$ . The "tubes"  $\tilde{\mathbf{A}}$  are "stacks" of initially contiguous material which "split" along the glide plane during slip. The extra half-plane for the positive edge segment of the dislocation is proportional to  $\mathbf{a}_y \wedge \mathbf{a}_z$ ; when this plane glides the Burgers vector passes over part of  $\vec{\mathbf{A}}$  through tubes  $\tilde{\mathbf{A}}$ . Atoms in this extra half-plane pass through "tubes"  $\mathbf{a}^y \wedge \mathbf{a}^z$  "pointing" in the  $x$ -direction at a velocity  $\mathbf{v} = v^x \mathbf{a}_x$ , but all other atoms are stationary. The right-hand screw segments passes through an area proportional to  $\mathbf{a}_x \wedge \mathbf{a}_z$ , while for the left-hand screw segment this area is  $-\mathbf{a}_x \wedge \mathbf{a}_z = \mathbf{a}_z \wedge \mathbf{a}_x$ .

A dislocation loop shaped like a parallelogram has edge segments characterized by the vector  $\mathbf{e} = e^m \mathbf{a}_m$ , and  $\mathbf{s} = s^m \mathbf{a}_m$  for the screw segments. Components of the unit vector  $\xi$  along the dislocation axis can be used to write  $e^m$  and  $s^m$  as  $e^m \equiv e\xi^m$ , and  $s^m \equiv s\xi^m$ ; for Figure 31,  $e^y = e\xi^y$  and  $s^x = s\xi^x$ . Dislocation glide over the slip plane  $\vec{\mathbf{A}} \equiv A\mathbf{a}_x \wedge \mathbf{a}_y$  occurs when  $\pm$ edge segments of the loop move by  $n^x$  steps in the direction  $\pm\mathbf{b}$  and screw segments move by  $n^y$  steps perpendicular (crystallographically) to  $\mathbf{b}$ . If dislocation motion is unimpeded, then  $n^x = n^y \equiv n$ . Edge segment lines cross over area  $\mathbf{e} \wedge n^x \mathbf{a}_x = e^y \mathbf{a}_y \wedge n^x \mathbf{a}_x = e\xi^y n^x \mathbf{a}_y \wedge \mathbf{a}_x \equiv l^{yx} \mathbf{a}_y \wedge \mathbf{a}_x$ ,  $l^{yx} \equiv e\xi^y n^x$ , and screw segment lines cross over area  $\mathbf{s} \wedge n^y \mathbf{a}_y = s^x \mathbf{a}_x \wedge \mathbf{a}_y = s\xi^x n^y \mathbf{a}_x \wedge \mathbf{a}_y \equiv l^{xy} \mathbf{a}_x \wedge \mathbf{a}_y$ ,  $l^{xy} \equiv s\xi^x n^y$ . The bivector  $\vec{l} = l^{mn} \mathbf{a}_m \wedge \mathbf{a}_n$  is the area ( $[\vec{l}] = \text{area}$ ) of the slip plane over which dislocation motion has occurred. For a loop

with  $e = s \equiv l$ :

$$\vec{l} \equiv l^{mn} \mathbf{a}_m \wedge \mathbf{a}_n = l \xi^m n^n \mathbf{a}_m \wedge \mathbf{a}_n.$$

#### 4.2.3. The Dislocation Movement Tensor

The bivector  $\vec{l}$  can be written as an "area 1-form"  $\tilde{l}$  (Nabarro 1967, Misner *et al.* 1973) with the "second notation":

$$\tilde{l} \equiv \tilde{l}_q \mathbf{a}^q \equiv \epsilon_{qmn} l^{mn} \mathbf{a}^q, \tilde{l}_q \equiv \epsilon_{qmn} l^{mn} \equiv \Omega e_{qmn} l^{mn};$$

$[\tilde{l}] = \text{area}$  and  $[\tilde{l}_q] = \text{volume}$ . An "incremental plastic shear",  $\Delta^{\mathcal{P}}\gamma_q^p$ , results when the dislocation moves over the slip plane by the amount  $\tilde{l} = \tilde{l}_q \mathbf{a}^q$  (Reed-Hill 1973):

$$\Delta^{\mathcal{P}}\gamma_q^p \equiv \tilde{l}_q b^p / \text{volume} \equiv \tilde{l}_q b^p / \Omega \gamma(x^m),$$

where  $\text{volume} \equiv \Omega \gamma(x^m) \equiv \gamma(x^a)$  is the volume of the complexion.

The *dislocation movement tensor* (Nabarro 1967) is

$$\mathcal{N} = \mathcal{N}^{mnp} \mathbf{a}_m \wedge \mathbf{a}_n \otimes \mathbf{a}_p, \mathcal{N}^{mnp} \equiv l^{mn} b^p / \Omega.$$

I have written  $\mathcal{N}$  as a *tensor density* (of weight  $-1$ ) by including  $\Omega$  in the definition;  $[\mathcal{N}] = 1$  and  $[\mathcal{N}^{mnp}] = \text{volume}^{-1}$ .<sup>[52]</sup> The plastic shear from dislocation movement is

[52]: So in an orthonormal frame,  $[\mathcal{N}^{abc}] = 1$ . Nabarro (1967) states that the dislocation density tensor  $\mathcal{N}^{abc}$  is a set of twenty-seven pure numbers in a discussion

$$\Delta^{\beta} \gamma_q^p = \frac{1}{2} \epsilon_{qmn} (\mathcal{N}^{mnp} - \mathcal{N}^{nmp}) / \gamma(x^m) = \frac{1}{2} \epsilon_{qmn} (l^{mn} - l^{nm}) b^p / \Omega \gamma(x^m).$$

Or, since  $\frac{1}{2} \epsilon_{qmn} (\mathcal{N}^{mnp} - \mathcal{N}^{nmp}) = \frac{1}{2} \epsilon_{qmn} \mathcal{N}^{mnp} - \frac{1}{2} \epsilon_{qnm} \mathcal{N}^{mnp} = \frac{1}{2} (\epsilon_{qmn} - \epsilon_{qnm}) \mathcal{N}^{mnp} = \epsilon_{qmn} \mathcal{N}^{mnp}$ ,

$$\Delta^{\beta} \gamma_q^p = \epsilon_{qmn} \mathcal{N}^{mnp} / \gamma(x^m) = \epsilon_{qmn} l^{mn} b^p / \Omega \gamma(x^m) = \epsilon_{qmn} l \xi^m n^n b^p / \Omega \gamma(x^m).$$

Glide of the screw segments corresponds to  $m \neq n = p$ ;  $p = m \neq n$  represents glide of the edge segments; and  $m \neq n \neq p$  is for climb of the edge segments.

The dislocation movement tensor describes the "*plastic history*" of "local regions" of the lattice (Nabarro 1967). It is therefore applicable to a complexion of corpuscles which deform by the same mechanism, and can be extended to the entire gauge length of the tensile specimen only when all complexions deform in the same way. If different complexions deform per different mechanisms, then some sort of "weighting" procedure must be employed to determine the strain rate. A simple procedure of this sort is described at the end of the next section. The following sub-section develops the Orowan equation for the case where a single deformation mechanism is operative.

***"Thus there is an enormous gap between the theory developed for the interaction between a few simple geometry dislocations and a description of macroscopic deformation"*** (Hirth and Lothe 1982).

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where his nomenclature suggests use of orthonormal coordinates.

#### 4.2.4. The Orowan Equation

Now assume that  $N$  dislocation loops of the same type are mobile. The quantity  $N[l\xi^m/\Omega\gamma(x^m)]$  is a measure of the dislocation density (Reed-Hill 1973), say

$$\bar{\rho}^m \equiv Nl\xi^m/\Omega\gamma(x^m), \quad \vec{\rho} \equiv \bar{\rho}^m \mathbf{a}_m. \quad \text{EQ 1}$$

The units of  $\vec{\rho} \equiv \bar{\rho}^m \mathbf{a}_m$  are  $[\vec{\rho}] = \text{dislocation length/volume}$ , and this is the measure used in the next section;  $[\bar{\rho}^m] = \text{volume}^{-1}$  for crystallographic coordinates and, for an orthonormal frame  $[\bar{\rho}^a] = \text{area}^{-1}$ . Thus,

$$\Delta^P\gamma_{q^p} = N[\epsilon_{qmn} l\xi^m n^n b^p/\Omega\gamma(x^m)] = \epsilon_{qmn} \bar{\rho}^m n^n b^p.$$

For *single glide*, with  $\mathbf{v} = v\mathbf{a}_x$  equal to the relative rate at which the lattice on opposite sides of the slip plane separate in Figure 31, segments of a dislocation loop travel as follows, assuming that motion is isotropic and unobstructed: ( $\pm$ ) edge segments have velocities  $\pm v^x \mathbf{a}_x \equiv \pm v\mathbf{a}_x$ ; the right-hand screw segment has velocity  $v^y \mathbf{a}_y = v\mathbf{a}_y$ , and the left-hand screw segment has velocity  $-v^y \mathbf{a}_y = -v\mathbf{a}_y$ . These velocities are given by  $v^m \equiv n^m/\Delta t$ . Therefore, since  $\Delta^P\gamma_{q^p} = \epsilon_{qmn} \bar{\rho}^m n^n b^p$ , the **Orowan equation** is

$$\Delta^P\gamma_{q^p}/\Delta t \equiv \dot{\gamma}_{q^p}^\bullet = \epsilon_{qmn} \bar{\rho}^m v^n b^p \equiv J_{q^p}, \quad \text{EQ 2}$$

where  $\dot{\gamma}_{q^p}^\bullet$  is the *plastic shear rate*, a Pfaffian,  $\dot{\gamma}_{q^p}^\bullet \equiv \dot{\gamma}_{q^p}^\bullet \mathbf{a}^q$ , and  $\mathbf{J}^p \equiv J_{q^p} \mathbf{a}^q$  are the dislocation

current 1-forms; see Kosevich (1979) as well. The dislocation current 1-form for Figure 31 is  $\mathbf{J}^x = J_z^x \mathbf{a}^z$ ; the planes  $\mathbf{a}^z$ , which are parallel to area  $\vec{\mathbf{A}} \equiv A \mathbf{a}_x \wedge \mathbf{a}_y$ , slip over  $\vec{\mathbf{A}}$ . For the  $\pm$  edge segments,  $J_z^x = \epsilon_{zyx} \vec{\rho}^y v^x b^x > 0$ , since  $\epsilon_{zyx} = -\Omega$ ,  $\vec{\rho}^y \propto \mp 1$ ,  $b^x = 1$ ,  $v^x = \pm v$ . For the screw segments,  $J_z^x = \epsilon_{zyx} \vec{\rho}^x v^y b^x > 0$ , since  $\epsilon_{zyx} = \Omega$ ,  $\vec{\rho}^y \propto \pm 1$ ,  $b^x = 1$ ,  $v^y = \pm v$ , for right-hand (+) and left-hand (—) segments, respectively.

The dislocation current 1-forms are  $\mathbf{J}^p \equiv J_q^p \mathbf{a}^q$ , with  $J_q^p \equiv \epsilon_{qmn} \vec{\rho}^m v^n b^p$ . The duals,  ${}^* \mathbf{J}^p$ , of the objects  $\mathbf{J}^p$  are the 2-forms

$$\begin{aligned} {}^* \mathbf{J}^p &= J^{qp} \epsilon_{qrs} \mathbf{a}^r \wedge \mathbf{a}^s = \epsilon^{qmn} \vec{\rho}_m v_n b^p \epsilon_{qrs} \mathbf{a}^r \wedge \mathbf{a}^s, \\ &= \epsilon^{qmn} \epsilon_{qrs} \vec{\rho}_m v_n b^p \mathbf{a}^r \wedge \mathbf{a}^s, \\ &= (\delta_m^r \delta_s^r - \delta_m^s \delta_r^s) \vec{\rho}_m v_n b^p \mathbf{a}^r \wedge \mathbf{a}^s, \\ &= (\vec{\rho}_r v_s - \vec{\rho}_s v_r) b^p \mathbf{a}^r \wedge \mathbf{a}^s, \\ &= 2 \vec{\rho}_r v_s b^p \mathbf{a}^r \wedge \mathbf{a}^s, \\ &\equiv (2b^p)^b \vec{\mathbf{p}} \wedge {}^b \mathbf{v}. \end{aligned}$$

For example, the positive edge dislocation flux through the "tubes"  $\tilde{\mathbf{A}} \equiv 2A^{-1} \mathbf{a}^x \wedge \mathbf{a}^y$  is the 2-form  ${}^* \mathbf{J}^x = 2 \vec{\rho}_y v_x b^x \mathbf{a}^y \wedge \mathbf{a}^x$ , which is positive, since  $\vec{\rho}_y < 0$ ,  $v_x > 0$ ,  $b^x > 0$ , and  $\mathbf{a}^y \wedge \mathbf{a}^x < 0$ . "Tubes"  $\tilde{\mathbf{A}}$  and "tubes"  ${}^* \mathbf{J}^x$  both "point" in the  $z$ -direction; the "tubes"  ${}^* \mathbf{J}^x$  "carry" an  $x$ -object,  $b^x$ .

### 4.3. Constitutive Relationships

*"The development of a comprehensive theory which describes the macroscopic behavior of real materials is extremely difficult. Such theories, if they are to be useful, must regard the material as a continuum. The major difficulty is the introduction of sensible constitutive relationships which describe the properties of the material. Indeed, one task of the materials scientist is to study the physical properties of materials in the hope that the microstructure can be understood and controlled in a way that improves the mechanical properties. The concept of a microstructure cannot easily be introduced when developing a continuum theory."* From McCartney (1980).

A constitutive relationship gives the stress (elastic and/or plastic) as a function of either the strain or the strain rate through a thermodynamic argument of some kind. McCartney (1981) derives constitutive relationships for creep deformation from "irreversible thermodynamics." See Malvern (1969) for a "standard" treatment of "irreversible thermodynamics" and constitutive relationships, and Lavenda (1978) for a more advanced treatment. Nabarro uses "irreversible thermodynamics" to describe dislocation motion in a crystal lattice, see the following box, and Edelen (1979) does the same using exterior calculus. Edelen also uses the theory to provide a constitutive relationship for plastic deformation from dislocation motion. Edelen's work is summarized here; his textbook

(Edelen 1985) discusses the theory of "irreversible thermodynamics" with exterior calculus. Lavenda (1978), Burke (1985), and Landsberg (1990) all use exterior calculus to describe "elementary" aspects of thermodynamics in their textbooks; Edelen's (1976) article on the subject is, on the other hand, quite advanced.

Ashby and Verrall (1973) develop a constitutive relationship for superplasticity by applying the theory of "irreversible thermodynamics" (Denbigh 1951) to the neighbor switching mechanism of superplastic flow (Lee 1970, McLean 1970). The neighbor switching mechanism of superplastic deformation is addressed in the following section. Morral and Ashby (1974) adapt the neighbor switching mechanism for the translatory grain movements (Rachinger 1952-53) which must be responsible for superplastic flow in a manner equivalent to crystal slip by suggesting that grain movements occur at cellular dislocations. Sherwood and Hamilton (1994) borrow "irreversible thermodynamics" from Nabarro (1967), Christian (1965), and Ashby and Verrall (1973), to cast Morral and Ashby's theory into a form consistent with Nabarro (1967) and Christian (1965). After reading Lavenda (1978), I think that a constitutive relationship for plastic deformation (of any kind) based upon "irreversible thermodynamics" is likely to be "semi-empirical."

This sub-section provides background material for some of the relationships cited in the next section.

### **Nabarro's (1967) Treatment of Energy Dissipation from Dislocation Motion**

There are at least four mechanisms by which atomic dislocations dissipate energy in a crystal lattice during plastic deformation at low homologous temperatures:

- (1) moving dislocations acquire a large kinetic energy that is released when they are stopped;
- (2) thermoelastic damping, radiation damping, and scattering of sound waves;
- (3) creation and annihilation of dislocation lines; and
- (4) creation and annihilation of point defects.

Mechanism 2 is addressed here.

Consider a screw dislocation moving in a slip plane travelling at velocity  $v$  in a medium with viscosity  $\eta$ ; its displacement and velocity are  $w = (b/2\pi)\tan^{-1}[y/(x - vt)]$  and  $\partial w/\partial t \equiv w_t = (bv/2\pi)[y/(x - vt)^2 + y^2]$ , respectively. The rate that energy is dispersed into unit volume, say  $\zeta$ , is  $\zeta = \frac{1}{2}\eta[(\partial w_t/\partial x)^2 + (\partial w_t/\partial y)^2] = b^2 v^2 \eta / 8\pi^2 r^4$ , where  $r \equiv [x^2 + y^2]^{1/2}$ . Per unit dislocation length, this quantity becomes  $\zeta_t = b^2 v^2 \eta / (8\pi r_o^2)$ ,  $r_o$  denoting the dislocation "core radius." Equating  $\zeta_t$  to the power supplied by the external shear stress ( $\tau$ ) to unit length of the dislocation, say  $P_t$ ,  $P_t = \tau b v$ ,  $\tau = bv\eta / (8\pi r_o^2)$  is obtained. Here,  $F_t = \tau b$  is the Peach-Koehler "force" that overcomes the viscous drag  $R_t v$  per unit length, where  $R_t \equiv (b^2/8\pi r_o^2)\eta$  is the *phonon resistivity*. Therefore  $v = R_t^{-1} \tau b$ ,  $R_t^{-1}$  denoting the dislocation mobility, say  $M$ ,  $M \equiv R_t^{-1}$ , so finally  $v = M\tau b$ .



Plastic deformation is subject to the following three *constraints*:

- (1) Balance of moment of momentum,
- (2) Balance of energy,
- (3) Constancy of volume.

These are discussed in turn.

**Balance of Moment of Momentum:** Let  $f^m$  denote components of the externally applied body force per unit mass ( $m$  is the mass density) and let

$$\sigma^m = \frac{1}{2} \epsilon_{MNP} \sigma^{Mm} \vec{d}X^N \wedge \vec{d}X^P$$

be the *Piola-Kirchoff* stress that balances the resultant tractions. It is antisymmetric but the corresponding Cauchy stress tensor is symmetric to balance the moment of momentum;  $[\sigma^m] = \text{force/area}$ . The *balance of linear momentum* is  $\partial_t \int_V m v^m \epsilon = \int_{\partial V} \sigma^m + \int_V m f^m \epsilon = \int_V (\vec{d}\sigma^m + m f^m \epsilon)$ , the last equality following from Stokes' theorem; here,  $\partial_t \equiv \partial/\partial t$ ,  $v^m \equiv \partial_t \chi^m$ , where  $\chi^m$  are functions giving the coordinates  $x^m$  of the material's boundary, and  $\epsilon = \vec{d}X \wedge \vec{d}Y \wedge \vec{d}Z$ . Since  $\partial_t m \epsilon = \mathbf{0}$ ,  $m \partial_t v^m \epsilon = \vec{d}\sigma^m + m f^m \epsilon$ , or in components,  $m \partial_t v^m = \partial_M \sigma^{Mm} + m f^m$ . *Balance of the moment of momentum* is represented by the integral  $\partial_t \int_V m \chi^n v^m \epsilon = \int_{\partial V} \chi^n \sigma^m + \int_V m \chi^n f^m \epsilon$  which, with  $m \partial_t v^m = \partial_M \sigma^{Mm} + m f^m$ , gives

$$(\partial_M \chi^n) \sigma^{Mm} = (\partial_M \chi^m) \sigma^{Mn}.$$

**Balance of Energy:** Let  $r$  denote the *rate of external energy supply* per unit mass of the reference configuration,  $\mathbf{q} = \frac{1}{2}\epsilon_{MNP} q^M \vec{d}X^N \wedge \vec{d}X^P$  denote the 2-form of *heat influx*, and  $E$  the *internal energy* per unit mass. The *balance of energy* is  $\partial_t \int_V m(\frac{1}{2}v^m \delta_{mn} v^n + E) \epsilon = \int_{\partial V} (v^m \delta_{mn} \sigma^n - \mathbf{q}) + \int_V m(v^m \delta_{mn} f^n + r)$ , which with Stokes' theorem is

$$m\partial_t E \epsilon = \delta_{mn} \sigma^m \wedge \vec{d}v^n - \vec{d}\mathbf{q} + mr\epsilon,$$

or in components  $m\partial_t E = \delta_{mn} \sigma^{Mm} \partial_M v^n - \partial_M q^M + mr$ .

**Constancy of Volume:** Plastic deformation is a constant volume process. Therefore  $\gamma_x^m + \gamma_y^m + \gamma_z^m = 0 \Rightarrow \partial_t \gamma_x^m + \partial_t \gamma_y^m + \partial_t \gamma_z^m = 0$ . Edelen (1979) writes the latter compactly as

$$X^M J_M^m = \mathbf{0}.$$

A *deterministic theory* results when  $\{\mathbf{J}^m, \sigma^m, \mathbf{q}, E\}$  are specified subject to the *constraints* of constant volume, balance of moment of momentum, and balance of energy, which are respectively:

$$X^M J_M^m = \mathbf{0}, \quad \sigma^{Mm} \partial_M \chi^n = \sigma^{Mn} \partial_M \chi^m, \quad m\partial_t E = \delta_{mn} \sigma^{Mm} \partial_M v^n - \partial_M q^M + mr.$$

The mechanical state of a dislocated body is described by the *external state variables*  $\chi^m$  and  $v^m$ , describing the external configuration and velocity of the body, respectively, and the *internal state variables*  $\gamma_M^m$  and  $\rho^{Mm} \equiv \epsilon^{MPQ} \partial_P \gamma_Q^n = \frac{1}{2} \epsilon^{MPQ} T^n_{PQ}$ . At any instant a *non-*

*equilibrium state* is approximated by a *constrained equilibrium state* which utilizes the same values of these variables for the internal energy  $E$ , and additionally the *entropy*,  $S$ ,  $T = \partial E / \partial S$ , where  $T$  is the temperature:  $E = E(\rho^{Mm}, \chi^m, \gamma_{Mm}, \mathcal{E}_{MN}, S)$ . The stress  $\sigma^{Mm}$  is just a function of the strain

$$\mathcal{E}_{MN} = \frac{1}{2} [(\partial_M \chi^m) \delta_{mn} (\partial_N \chi^n) - \delta_{MN}]$$

for crystalline materials:

$$\sigma^{Mm} = m (\partial E / \partial \mathcal{E}_{MN}) \partial_N \chi^m.$$

For viscoelastic materials or fluids the stress is also a function of a "*dissipative stress*", say

$$\mathcal{T}_m^M,$$

$$\sigma^{Mm} = \delta^{mn} [\mathcal{T}_n^M + m (\partial E / \partial \mathcal{E}_{MN}) \partial_N \chi^m],$$

and this should also be the case for cellular dislocations in a polycrystalline material. The energy equation  $m \partial_t E = \delta_{mn} \sigma^{Mm} \partial_M v^n - \partial_M q^M + mr$ , with

$$E = E(\partial_M \chi^m, \gamma_{Mm}, \rho^{Mm}, \chi^m),$$

can therefore be rewritten using the chain rule for differentiation (with respect to time  $t$ ):

$$\begin{aligned} m T \partial_t S + [\partial E / \partial (\partial_M \chi^m)] \partial_M v^m + [\partial E / \partial \gamma_{Mm}] \partial_t \gamma_{Mm} + [\partial E / \partial \rho^{Mm}] \partial_t \rho^{Mm} \\ = \delta_{mn} \sigma^{Mn} \partial_M v^n - \partial_M q^M + mr. \end{aligned}$$

Using the expressions  $\mathbf{J}^m = J_{M^m} \vec{\mathbf{d}}X^M = -[\partial(\gamma_{M^m})/\partial t] \vec{\mathbf{d}}X^M$  and  $\partial \tilde{\mathbf{p}}^m / \partial t = -\vec{\mathbf{d}}\mathbf{J}^m = -(\partial J_{M^m} / \partial X^N) \vec{\mathbf{d}}X^N \wedge \vec{\mathbf{d}}X^M$ , the former expression can be rewritten to give the "final balance equation":

$$\begin{aligned} m\partial_t S + \partial_M [q^M/T + m\epsilon^{MNP}(\partial E/\partial\rho^{Nm})J_{P^m}/T] - mr/T &= T^{-1} [\delta_{mn} \sigma^{Mn} - m\partial E/\partial(\partial_M \chi^m)] \partial_M v^m \\ &\quad + m/T [\partial E/\partial\gamma_{M^m} - \epsilon^{MNP} \partial_N (\partial E/\partial\rho^{Pm})] J_{M^m} \\ &\quad - T^{-2} [q^M + m\epsilon^{MNP}(\partial E/\partial\rho^{Nm})J_{P^m}] \partial_M T. \end{aligned}$$

Edelen refers to the term  $(q^M + m\epsilon^{MNP}(\partial E/\partial\rho^{Nm})J_{P^m})/T$  as the (components of) *entropy influx 2-form*:

$$\begin{aligned} \eta &\equiv \frac{1}{2} \eta^M \epsilon_{MNP} \vec{\mathbf{d}}X^N \wedge \vec{\mathbf{d}}X^P, \\ \eta^M &\equiv (q^M + m\epsilon^{MNP}(\partial E/\partial\rho^{Nm})J_{P^m})/T. \end{aligned}$$

Components  $\eta^M$  of the entropy influx  $\eta$  are proportional to the sum of the heat influx  $q^M$  and the term  $m\epsilon^{MNP}(\partial E/\partial\rho^{Nm})J_{P^m}$ ; the latter represents a *mode of heat addition* arising from the *internal degrees of freedom* of the material, *i.e.* the dislocations. The "entropy production rate",<sup>[53]</sup>  $\theta$ , is just the right-hand side of the "final balance equation":

[53]: Malvern (1969) defines the *local entropy production*,  $\theta$ , as

$$\theta \equiv dS/dt - r/T + (mT)^{-1} \nabla \cdot \vec{\mathbf{q}},$$

with  $\vec{\mathbf{q}}$  denoting the *heat flux vector*, *e.g.*  $\vec{\mathbf{q}} \equiv -k\nabla T$ , where  $k$  is the *thermal conductivity* of the material.

$$\begin{aligned}\theta \equiv & T^{-1}[\delta_{mn}\sigma^{Mn} - m\partial E/\partial(\partial_M\chi^m)]\partial_M v^m + m/T[\partial E/\partial\gamma_{M^m} - \epsilon^{MNP}\partial_N(\partial E/\partial\rho^{Pm})]J_M{}^m \\ & - T^{-2}[q^M + m\epsilon^{MNP}(\partial E/\partial\rho^{Nm})J_P{}^m]\partial_M T.\end{aligned}$$

Variables occurring in this expression for the entropy production rate  $\theta$  can be partitioned into sets of *thermodynamic forces*, say  $\mathcal{E}^M{}_m$ , and associated *thermodynamic fluxes*,  $J_M{}^m$  and  $j^M$ , such that

$$T\theta = \mathcal{T}^M{}_m\partial_M v^m + J_M{}^m\mathcal{E}^M{}_m + T^{-1}j^M\partial_M T \geq 0$$

is the *dissipation inequality*. Here,

$$\mathcal{E}^M{}_m = m[\partial E/\partial\gamma_{M^m} + \epsilon^{MNP}\partial_N(\partial E/\partial\rho^{Pm})],$$

and

$$j^M \equiv -\{q^M + m\epsilon^{MNP}[\partial_N(\partial E/\partial\rho^{Nm})]J_P{}^m\}.$$

The dissipation inequality is solved for the quantities  $\{\mathcal{T}^M{}_m, J_M{}^m, j^M\}$  subject to the constraints

$X^M J_M{}^m = 0$  and  $X^M \gamma_{M^m}$  for constancy of volume, and  $\sigma^{Mm}\partial_M\chi^m = \sigma^{Mn}\partial_M\chi^m$  for balance of moment of momentum.

Thermodynamic forces and fluxes vanish in any equilibrium state, and therefore  $\theta$  does too. So for any equilibrium state, the above relationships for the fluxes and forces set equal to zero result in the list

**In an Equilibrium State:**

$$\partial_M v^m = \partial_M \partial_t \chi^m = 0, \quad \partial_M T = 0;$$

$$\partial E / \partial \gamma_M^m = -\epsilon^{MNP} \partial_N (\partial E / \partial \rho^P);$$

$$J_M^m = 0, \quad \mathcal{T}_m^M = 0, \quad j^M = 0;$$

$$\sigma^{Mm} = m(\partial E / \partial \varepsilon_{MN}) \partial_N \chi^m, \quad q^M = -m\epsilon^{MNP} [\partial_N (\partial E / \partial \rho^N)] J_P^m = 0.$$

This list indicates that in an equilibrium state there is no overall flow of energy across the system (tensile specimen) and no overall movement of the system (Denbigh 1951).

For the case of dislocation motion through a crystalline substance there is no dissipative stress,  $\mathcal{T}_m^M = 0$ , and the dissipation inequality reduces to  $T\theta = J_M^m \mathcal{E}_m^M \geq 0$ , which is subject to only the constraints  $J_M^m \chi^M = 0$ . Edelen's solution to this problem is

$$J_M^m = M^{mn} \partial_N (x^2 \mathcal{E}_n^N - x^p \mathcal{E}_n^Q \delta_{pq} x^Q),$$

where  $M^{mn} \partial_N$  represents entries in a positive definite  $9 \times 9$  matrix:

$$M^{mn} \partial_N = \begin{vmatrix} \|x_X\| & \|y_X\| & \|z_X\| \\ \|x_Y\| & \|y_Y\| & \|z_Y\| \\ \|x_Z\| & \|y_Z\| & \|z_Z\| \end{vmatrix}.$$

#### 4.3.1. Grain Boundary Movement

Christian (1965) utilizes an argument from "non-equilibrium thermodynamics" to describe grain boundary migration, after Machlin (1953). The differential (or 1-form) of the state function entropy,  $S$ , can be decomposed as

$$dS \equiv d_e S - d_i S,$$

where  $d_e S$  is the entropy exchanged between the system and surroundings and  $d_i S$  is the entropy produced in the system, both being Pfaffians (inexact 1-forms).<sup>[54]</sup> This is the way that the entropy balance equation is written in "*generalized thermodynamics*" (Lavenda 1978).<sup>[55]</sup> For irreversible processes at constant temperature and pressure the Gibbs free energy 1-form is

$$dG = dE + pdV - TdS \equiv dH - TdS = -Td_e S - TdS = -Td_i S,$$

$dH \equiv -Td_e S \equiv dE + pdV$  denoting the *enthalpy* 1-form. Note that  $[G] = \text{energy/atom}$  and similarly for the other quantities here. The rate at which entropy is produced in the system,  $\theta$ , is consequently

$$\theta \equiv d_i S / \Delta t = -T^{-1} \partial G / \partial t.$$

[54]: During a reversible process where an amount of heat  $\Delta q$  enters the system from the surroundings  $TdS = \Delta q = -Td_e S$ ; the entropy of the surroundings decreases.

[55]: The subject of "non-equilibrium thermodynamics" is quite controversial; see Lavenda's (1978) review.

For any process which does not occur too far away from equilibrium

$$TdS = dH - \mu_\alpha dn^\alpha = dH - dG,$$

where  $\mu_\alpha \equiv \partial G / \partial n^\alpha$  is the *chemical potential* of species  $\alpha$  which number  $n^\alpha$ . Then

$$\Xi_\alpha J^\alpha \equiv T\theta = -\mu_\alpha dn^\alpha/dt,$$

$$\Xi_\alpha \equiv -\mu_\alpha = -\partial G / \partial n^\alpha$$

denoting the "*generalized thermodynamic force*" and

$$J^\alpha \equiv dn^\alpha/dt$$

the conjugate "*thermodynamic flux*".

The *reaction* is  $\partial^i \alpha_i = 0$  for the  $\alpha_1, \alpha_2, \dots, \alpha_i, \dots$  species of which there are initially  $n^{\alpha_i}_0 \equiv n^{\alpha_i}(t=0)$  in the assembly so that  $\zeta \equiv (n^{\alpha_i} - n^{\alpha_i}_0)/\partial^i$  measures the amount of reaction. If  $\partial^i > 0$  for the reaction products, then  $\zeta > 0$  is the *degree of advancement*. Writing  $d\zeta = dn^{\alpha_i}/\partial^i = dn^{\alpha_1}/\partial^1 = dn^{\alpha_2}/\partial^2 = \dots$ , then  $T\theta = -\mu_\alpha dn^\alpha/dt$  becomes

$$T\theta = -\partial^i \mu_{\alpha_i} (d\zeta/dt) = -(d\zeta/dt) [\partial^1 \mu_{\alpha_1} + \partial^2 \mu_{\alpha_2} \dots + \partial^i \mu_{\alpha_i} + \dots].$$

Supposing that the free energy of activation is  $\Delta G^*$  per atom, then the forward rate of the

reaction is proportional to  $\exp(-\Delta G^*/kT)$  while the backward rate of reaction is proportional to  $\exp(-\Delta G^*/kT + \partial^i \mu_{\alpha_i}/kT)$ . The net rate of the reaction is therefore proportional to

$$\exp(-\Delta G^*/kT)[1 - \exp(\partial^i \mu_{\alpha_i}/kT)] \approx -\exp(-\Delta G^*/kT)[\partial^i \mu_{\alpha_i}/kT],$$

which is linear in  $-\partial^i \mu_{\alpha_i}$  only when the approximation holds, *i.e.* when the reaction is so close to equilibrium that  $-\partial^i \mu_{\alpha_i} < < kT$ . This approximation likely holds when transport phenomena in the solid state are treated as "generalized reactions", *e.g.* grain boundary migration during annealing (Christian 1965) and grain boundary migration/sliding during creep (Nabarro 1967, Poirier 1985). The quantity

$$-\partial^i \mu_{\alpha_i} \equiv -\Delta G$$

is the *affinity* of the reaction, a positive quantity ( $\partial^i \mu_{\alpha_i} < 0$ ) which measures the free energy difference between reactants and products,  $-\partial^i \mu_{\alpha_i} = \sum_{\text{reactants}} G - \sum_{\text{products}} G = -\Delta G$ .

**Grain Boundary Migration as a "Generalized Reaction":** If an element of a grain boundary has surface area  $O$  and radius of curvature  $\varrho$  then when it moves normal to itself (definition of grain boundary migration) through a distance  $\delta r$  the total Gibbs free energy change is

$$\delta G = O(2\Gamma/\varrho)\delta r,$$

$\Gamma$  denoting the grain boundary surface tension. The "generalized thermodynamic force" is

$\mathcal{E}_\alpha \equiv -\mu_\alpha = -\partial G/\partial n^\alpha$  and the "thermodynamic flux" is  $J^\alpha \equiv dn^\alpha/dt$ . Taking position  $r$  as the variable  $n^\alpha$ ,

$$\mathcal{E}_r = -\mu_r = -\partial G/\partial r = -O(2\Gamma/\varrho), \text{ and } J^r = dr/dt \equiv v_{\text{GBM}} < 0,$$

where  $v_{\text{GBM}}$  is the *grain boundary migration velocity* ( $[v_{\text{GBM}}] = \text{distance/time}$ ). The entropy production rate from grain boundary migration (Machlin 1953)  $\theta$  is therefore

$$T\theta = \mathcal{E}_\alpha J^\alpha = -[O(2\Gamma/\varrho)]v_{\text{GBM}} > 0;$$

$[T\theta] = \text{power}$ . Atomic motion is often used for the level of description:

$$T\theta \equiv -\partial G/\partial t = [\Omega 2\Gamma/\varrho] v_{\text{GBM}}/\delta \equiv \mathcal{E}_{\text{GBM}} J_{\text{GBM}},$$

where  $[T\theta] = \text{power/atom}$ ;  $v_{\text{GBM}}/\delta \equiv J_{\text{GBM}}$ ,  $\delta$  denoting the grain boundary "width," and  $v_{\text{GBM}} \equiv \|v_{\text{GBM}}\|$ ;  $\mathcal{E}_{\text{GBM}} \equiv \Omega 2\Gamma/\varrho$ , and  $[\mathcal{E}_{\text{GBM}}] = \text{force/atom}$ .

The theory (of "non-equilibrium thermodynamics") assumes that the "force" and "flux" are linearly related. The relationship

$$v_{\text{GBM}} = M_B F_{\text{GBM}}$$

is therefore possible. Here,  $M_B = (\Omega/\delta)m_B = (\Omega/\delta)D_B/kT$  is the *grain boundary mobility*,  $m_B \equiv D_B/kT$  denoting the atomic mobility in a grain boundary, and  $F_{\text{GBM}} \equiv 2\Gamma/\varrho$  is the "driving

"force" for grain boundary migration,  $[F_{\text{GBM}}] = \text{pressure}$ ; see also Verhoeven (1975). Other such relationships are, however, possible (Christian 1965, Gleiter and Chalmers 1972, Smith, Rae and Grovenor 1980).<sup>[56]</sup> The relationship  $v_{\text{GBM}} = M_B F_{\text{GBM}}$  can be used to write the *grain growth rate*,  $\partial\mathbf{d}/\partial t$ ,  $\mathbf{d}$  denoting the average grain size, by identifying, rather crudely,  $\partial\mathbf{d}/\partial t$  with  $v_{\text{GBM}}$ :  $\partial\mathbf{d}/\partial t \equiv v_{\text{GBM}}$  (Christian 1965).

Hillert (1965) employs a different level of description for his "*defect theory*" of grain growth. The grain growth rate from Hillert's grain growth "reaction," or cellular dislocation climb (Cahn and Padawer 1965, Morral and Ashby 1974), is

$$\partial\mathbf{d}/\partial t = M_B [^{1/3}X_d(2\Gamma/\mathbf{d})],$$
[56]

$X_d$  denoting the fraction of non-hexagonal cells, which is proportional to the cellular dislocation density. Hillert's theory directly addresses the fact that **grain growth occurs because grains disappear from the microstructure** during, for example, annealing. His grain growth rate is derived next.

A cell with  $n \equiv (6 - p)$  neighbors is assumed to require a period of time  $\tau_p$  to disappear. The number of cells per unit volume,  $N_v$ , decays at a rate

$$dN_v/dt = -\sum_{p \leq 3} [f_p/\tau_p] N_v,$$

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[56]: And with respect to grain growth, see Abbruzzese and Lücke (1986), and Eichelkraut, Abbruzzese and Lücke (1988).

assuming first-order reactions kinetics, where  $f_p$  is the fraction of cells in the array with  $n = (6 - p)$  neighbors. An  $n = (6 - p)$ -sided cell shrinks at a rate  $\partial d_n / \partial t = -4p\Gamma M_B/(6d_n)$ ;

$$-\int_d^0 d_n dd_n = \frac{2}{3}p\Gamma M_B \int_0^{\tau_p} dt \Rightarrow \tau_p = 3(d/2)^2/(p\Gamma M_B),$$

where  $d$  is the average grain size. In two dimensions  $N_v d^2 = constant$  because cells fill all space in the array; therefore  $2(d\mathbf{d})/\mathbf{d} + (dN_v)/N_v = 0$ , or  $2(\partial \mathbf{d}/\partial t)/\mathbf{d} = -(\partial N_v/\partial t)/N_v$ ; thus,

$$\partial \mathbf{d}/\partial t = \frac{1}{2}\mathbf{d} \sum_{p \leq 3} [f_p/\tau_p] = \frac{1}{2}\mathbf{d} \sum_{p \leq 3} \{f_p/[3(d/2)^2/(p\Gamma M_B)]\} = 2 \sum_{p \leq 3} \{[pf_p](\Gamma M_B/3d)\} \equiv 2X_d(\Gamma M_B/3d),$$

where the *defect fraction* of the cellular array is,

$$X_d \equiv \sum_{p \leq 3} pf_p;$$



it counts only the non-hexagonal cells in an array, since for  $n = 6$  (a hexagon),  $p = 0$ .

**Grain Boundary Sliding/Migration as a "Generalized Reaction":** An element of a grain boundary moves tangential to itself during grain boundary sliding, for example, when neighbor switching occurs under the influence of an applied stress  $\sigma$ , which is the flow stress for superplastic or creep deformation. Ashby and Verrall (1973) assume that  $dS \equiv d_i S - d_e S = 0 \Rightarrow d_i S = d_e S = -\Delta q > 0$  for the neighbor switching "reaction." The initial and final states of this "reaction" are identical aside from relative cell translations and rotations

(discussed in the next section) and, consequently, state functions are stationary, *e.g.*  $dS = 0$  and  $dE = 0$ . Since  $dE = \Delta W + \Delta q = 0$ ,  $\Delta W = -\Delta q = d_i S$ , where  $\Delta W = \sigma \varepsilon_o$ ,  $\varepsilon_o = 0.55$  denoting the strain required for four cells to switch neighbors. Thus, on average,

$$\dot{W} = \frac{1}{2} \sigma \dot{\varepsilon} = T \theta;$$

where  $\dot{W} = \Delta W / \Delta t$  is the power input,  $P_{in}$ , to a unit volume of the material;  $\dot{\varepsilon}$  is the imposed strain rate, assumed to be picked up entirely by neighbor switching;  $\theta$  is the entropy production from all of the elementary processes required to "drive" the "reaction" (atomic diffusion, interface reaction, grain boundary sliding, grain boundary migration); and the factor of one-half is a *Schmid factor*. Thus, all of the power input to the material is assumed to be dissipated.

Cellular dislocation glide is the most efficient means of dissipating shear energy in a cellular array (Rivier *et al.* 1986). Sherwood and Hamilton (1994) borrow Nabarro's (1967) argument for lattice dislocation motion and write, after Morral and Ashby (1974)

$$v = \mathbf{M} \mathcal{E} \equiv \mathbf{M} \mathbf{b} \tau$$



for the cellular dislocation velocity  $v$ . Here,  $\mathbf{M}$  is the *cellular dislocation mobility*,  $\mathbf{b}$  is the Burgers vector,  $\tau$  is the resolved stress on the cellular dislocation, and  $\mathcal{E} \equiv \mathbf{b} \tau$  is the Peach Koehler (1950) "force" on the cellular dislocation. This relationship is used with the Orowan

equation in the next section to write the constitutive relationship for superplastic deformation.

Ducheyne and De Meester (1974) suggest that deformation-enhanced grain growth is an irreversible process driven by the applied stress. Sherwood and Hamilton (1994) describe this thought with stress-driven cellular dislocation climb.